LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 4922A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.095	12	18	37	rVB	525280	1062464	12.09%	2.211%
2	4.123	183	193	203	rBV3	50553	129366	1.47%	0.269%
3	4.957	318	335	347	rBV3	59812	260113	2.96%	0.541%
4	5.104	347	360	368	rBV4	40679	128451	1.46%	0.267%
5	5.556	427	437	442	rVV2	182891	374318	4.26%	0.779%
6	5.603	442	445	458	rVB2	67045	155672	1.77%	0.324%
7	7.166	689	711	723	rBV3	188278	709671	8.07%	1.477%
8	7.430	751	756	763	rVV	77062	125139	1.42%	0.260%
9	7.512	763	770	777	rVV4	75082	215366	2.45%	0.448%
10	7.759	807	812	817	rBV	71795	117351	1.34%	0.244%
11	7.912	830	838	841	rBV3	47458	101476	1.15%	0.211%
12	7.982	841	850	856	rVV4	110732	312071	3.55%	0.649%
13	8.047	856	861	868	rVV3	70976	174927	1.99%	0.364%
14	8.129	870	875	887	rVB5	72146	197943	2.25%	0.412%
15	8.288	893	902	913	rBV6	85851	220453	2.51%	0.459%
16	8.769	955	984	990	rBV2	262304	960148	10.92%	1.998%
17	9.110	1029	1042	1044	rBV7	108799	373114	4.25%	0.776%
18	9.145	1044	1048	1054	rVV	290280	574310	6.53%	1.195%
19	9.210	1054	1059	1068	rVB3	93475	205107	2.33%	0.427%
20	9.733	1086	1148	1149	rBV3	802199	8788996	100.00%	18.289%
21	9.956	1173	1186	1189	rBV	482998	1580562	17.98%	3.289%
22	10.109	1202	1212	1216	rVB3	466030	1279128	14.55%	2.662%
23	10.203	1222	1228	1243	rVB4	53349	122456	1.39%	0.255%
24	10.408	1243	1263	1267	rBV2	347827	1223912	13.93%	2.547%
25	10.467	1270	1273	1278	rVV2	68447	103951	1.18%	0.216%
26	10.543	1278	1286	1291	rVV3	111853	242008	2.75%	0.504%
27	10.608	1291	1297	1306	rVB2	148718	283774	3.23%	0.591%
28	10.737	1306	1319	1325	rBV2	265249	857206	9.75%	1.784%
29	10.796	1325	1329	1331	rVV	162158	277620	3.16%	0.578%
30	10.837	1332	1336	1347	rVV2	269307	574455	6.54%	1.195%
31	10.984	1347	1361	1368	rVB2	328665	1021561	11.62%	2.126%
32	11.295	1380	1414	1418	rBV6	523354	3630638	41.31%	7.555%
33	11.342	1418	1422	1427	rVB	230877	362470	4.12%	0.754%
34	11.466	1427	1443	1454	rVB3	582388	2149665	24.46%	4.473%
35	11.577	1456	1462	1464	rBV	144456	247200	2.81%	0.514%
36	11.818	1490	1503	1513	rVV3	548922	1797949	20.46%	3.741%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 4922A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.906	1514	1518	1522	rVV2	98412	193246	2.20%	0.402%
38	11.959	1522	1527	1536	rVV2	193321	359090	4.09%	0.747%
39	12.135	1548	1557	1562	rVB2	94337	206080	2.34%	0.429%
40	12.206	1564	1569	1573	rBV	82907	129802	1.48%	0.270%
41	12.282	1577	1582	1590	rVB3	130395	259044	2.95%	0.539%
42	12.458	1604	1612	1621	rVB	214814	478586	5.45%	0.996%
43	13.017	1691	1707	1717	rBV	510513	1544963	17.58%	3.215%
44	13.246	1740	1746	1752	rBV	674887	1047330	11.92%	2.179%
45	13.304	1752	1756	1764	rVB	63314	93235	1.06%	0.194%
46	13.439	1774	1779	1789	rVB2	182009	288822	3.29%	0.601%
47	13.604	1798	1807	1813	rBV	191781	358076	4.07%	0.745%
48	14.092	1881	1890	1896	rBV	396378	839689	9.55%	1.747%
49	14.509	1957	1961	1967	rVV	139820	187988	2.14%	0.391%
50	14.620	1975	1980	1988	rVB	263520	440205	5.01%	0.916%
51	14.943	2030	2035	2044	rBV4	43624	110310	1.26%	0.230%
52	15.460	2118	2123	2128	rVB	160621	210902	2.40%	0.439%
53	15.866	2183	2192	2196	rBV2	53748	122861	1.40%	0.256%
54	16.118	2230	2235	2241	rVB	453710	673847	7.67%	1.402%
55	16.318	2264	2269	2272	rBV	204507	283082	3.22%	0.589%
56	16.770	2342	2346	2352	rVB4	75831	123677	1.41%	0.257%
57	16.829	2352	2356	2365	rBV2	65036	120885	1.38%	0.252%
58	17.111	2400	2404	2409	rBV2	205401	263621	3.00%	0.549%
59	17.164	2409	2413	2418	rVB	103612	142620	1.62%	0.297%
60	17.369	2443	2448	2453	rBV	247776	378831	4.31%	0.788%
61	17.851	2526	2530	2537	rVB	190499	243618	2.77%	0.507%
62	18.027	2556	2560	2566	rVB2	96100	132747	1.51%	0.276%
63	18.268	2594	2601	2610	rBV	614771	1046300	11.90%	2.177%
64	18.480	2633	2637	2643	rBV	215789	321900	3.66%	0.670%
65	18.538	2644	2647	2652	rVB	153361	193511	2.20%	0.403%
66	19.167	2751	2754	2759	rBV	127135	150538	1.71%	0.313%
67	19.390	2787	2792	2795	rBV	286553	499625	5.68%	1.040%
68	19.531	2812	2816	2821	rBV	326231	410967	4.68%	0.855%
69	19.743	2849	2852	2856	rBV	115667	144560	1.64%	0.301%
70	19.978	2887	2892	2897	rVB	1032479	1319159	15.01%	2.745%
71	20.277	2940	2943	2947	rVB2	115397	126007	1.43%	0.262%
72	21.640	3172	3175	3183	rVB2	273386	435307	4.95%	0.906%
73	22.004	3233	3237	3246	rVB	277313	561768	6.39%	1.169%
74	22.398	3299	3304	3316	rVB	267976	782803	8.91%	1.629%
75	22.756	3359	3365	3382	rVB2	548950	1888700	21.49%	3.930%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

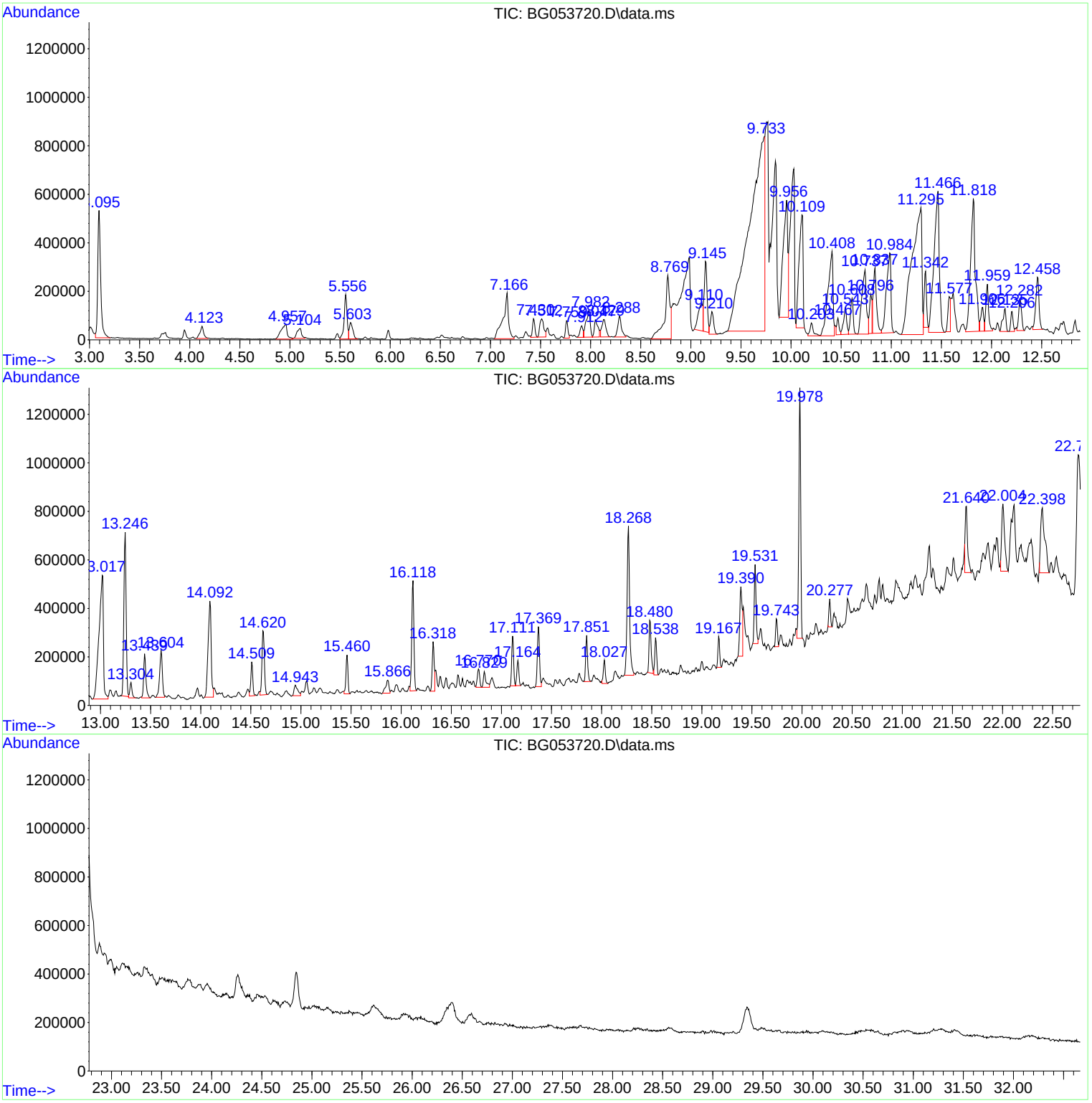
Sum of corrected areas: 48055313

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

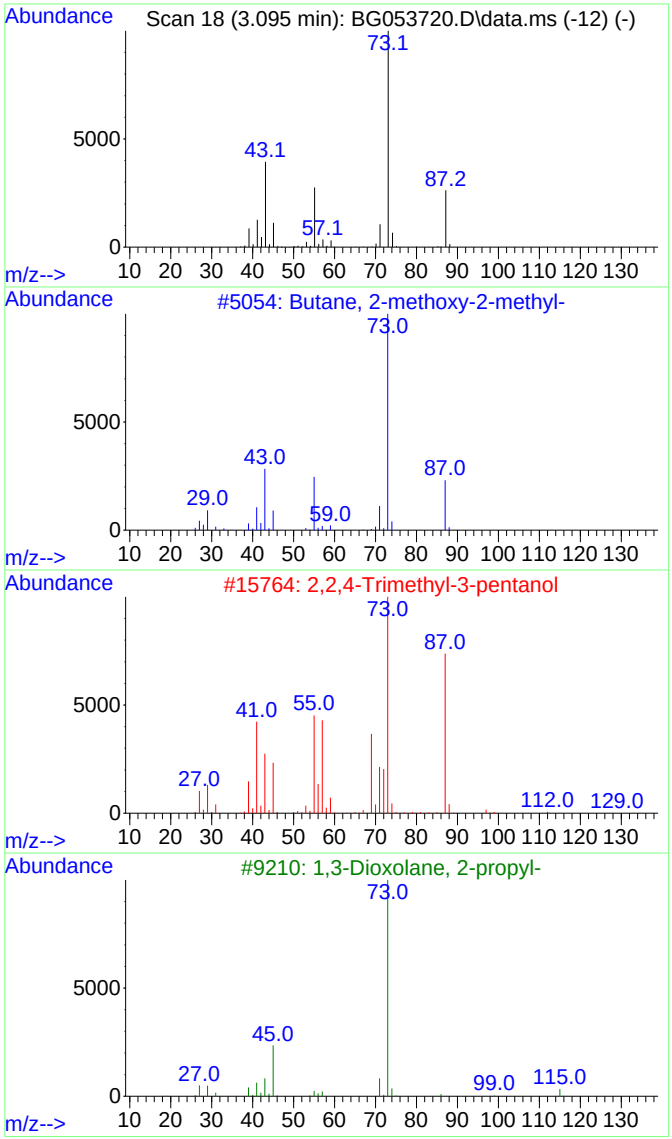
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

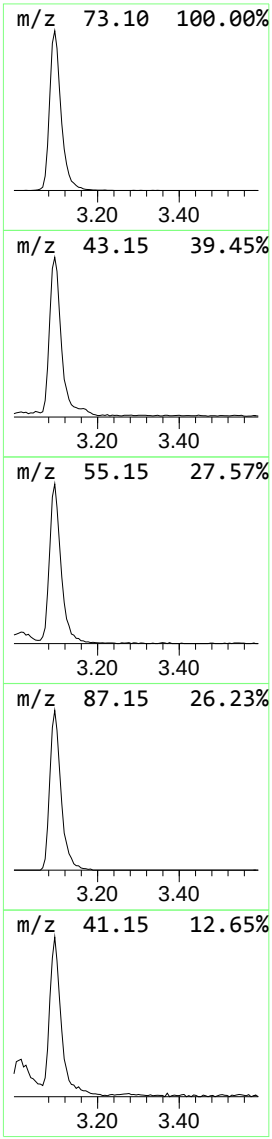
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.095	68.09 ng	1062460	1,4-Dichlorobenzene-d4	7.982

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

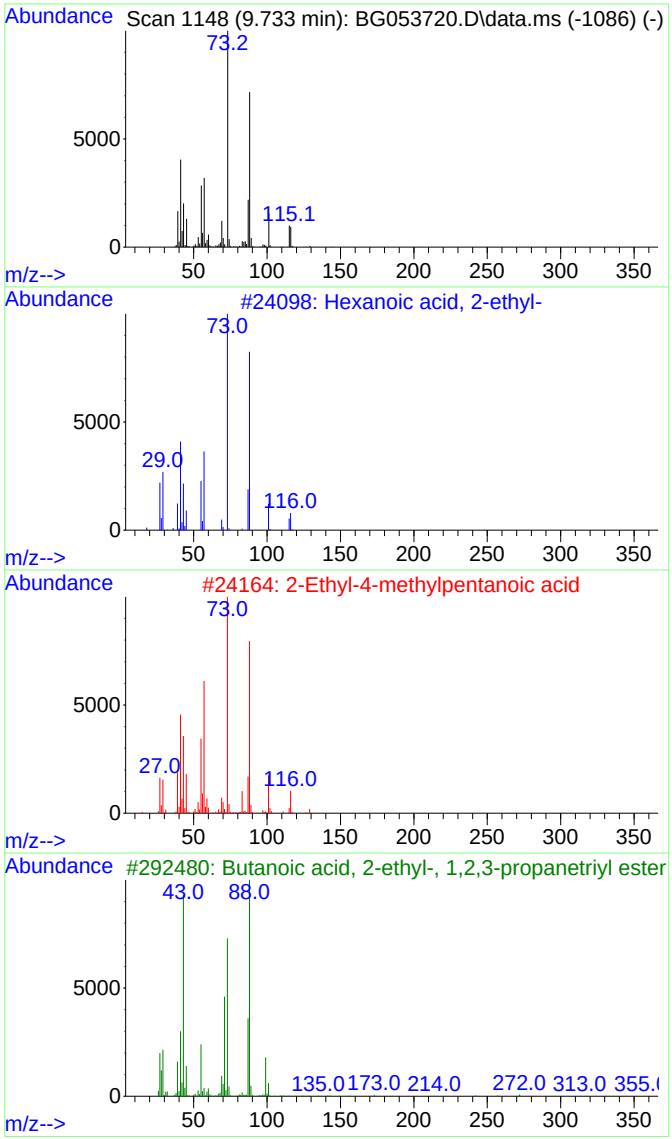
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

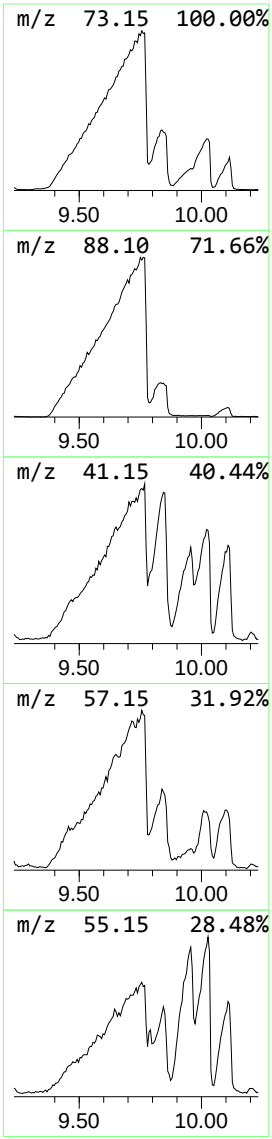
****

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	633.17 ng	8789000	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
4	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	43
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

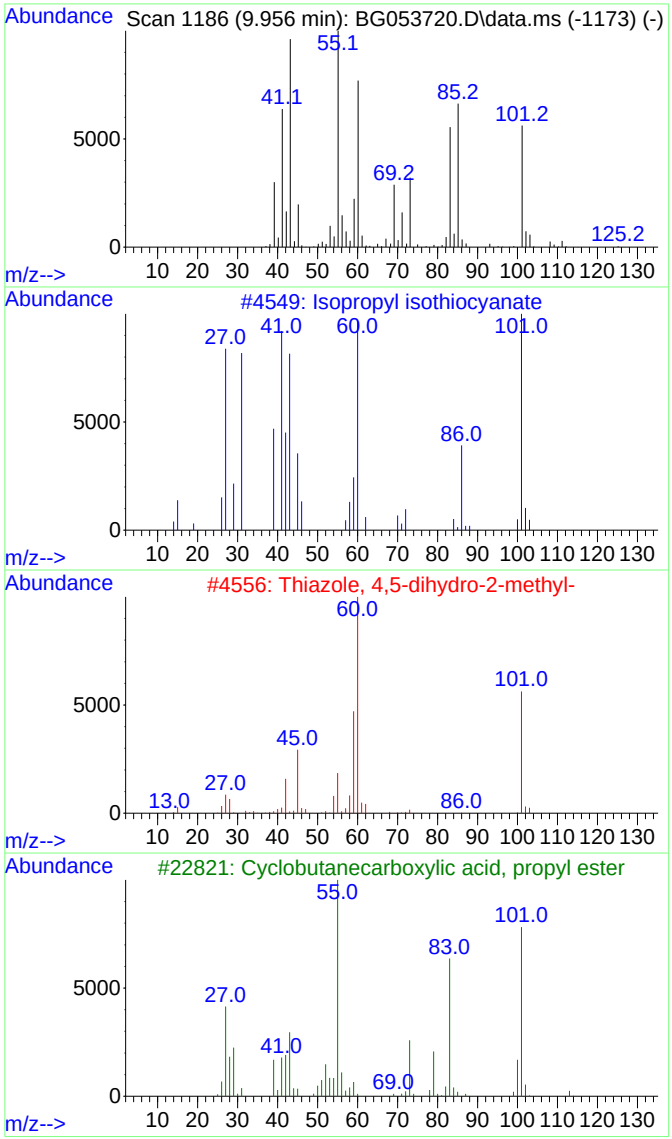
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

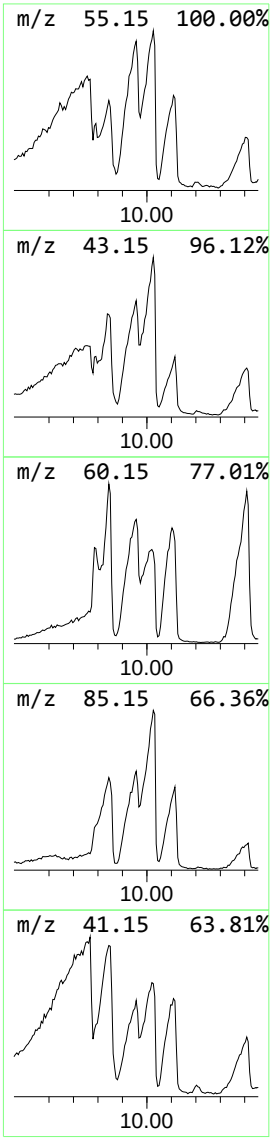
****

Peak Number 3 unknown9.956 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.956	113.86 ng	1580560	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	46
2	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	32
3	Cyclobutanecarboxylic acid, prop...	142	C8H14O2	1000280-40-0	27
4	Butanoic acid	88	C4H8O2	000107-92-6	16
5	Rhamnose	164	C6H12O5	003615-41-6	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

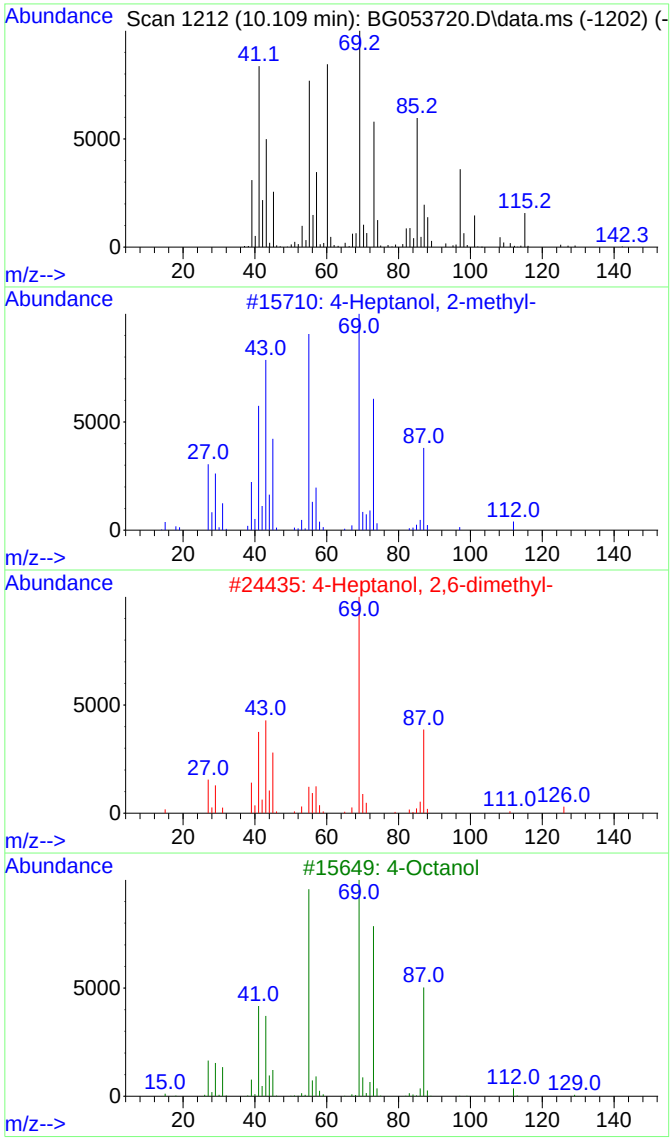
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

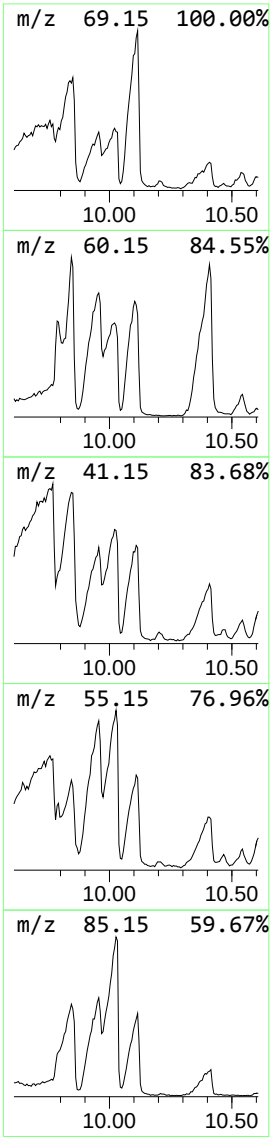
****

Peak Number 4 unknown10.109 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.109	92.15 ng	1279130	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2-methyl-	130	C8H18O	021570-35-4	35
2	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	27
3	4-Octanol	130	C8H18O	000589-62-8	27
4	Glutaric acid, 3-methylbut-2-en-...	282	C16H26O4	1000394-02-5	25
5	1,3-Dioxan-4-one, 2-(1-methyleth...	158	C8H14O3	1000197-64-0	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

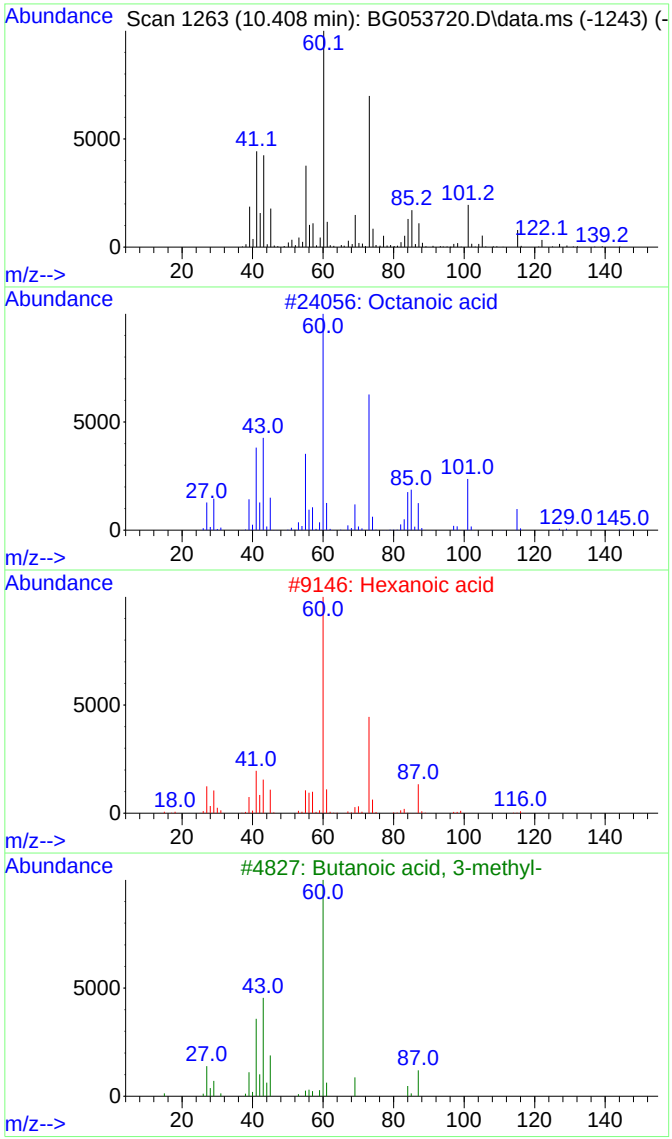
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

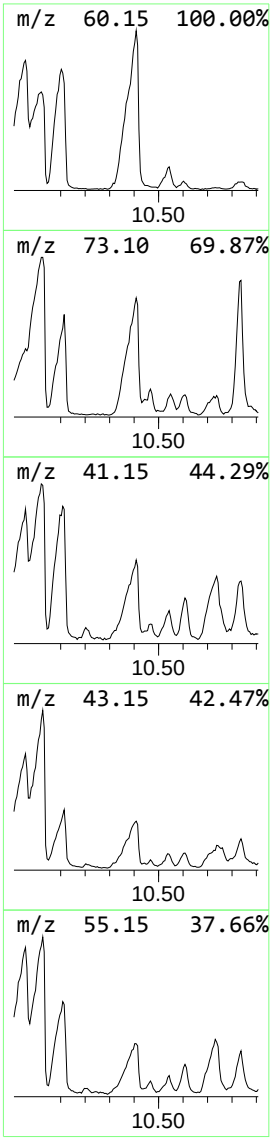
****

Peak Number 5 Octanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.408	88.17 ng	1223910	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	95
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	Butanoic acid	88	C4H8O2	000107-92-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

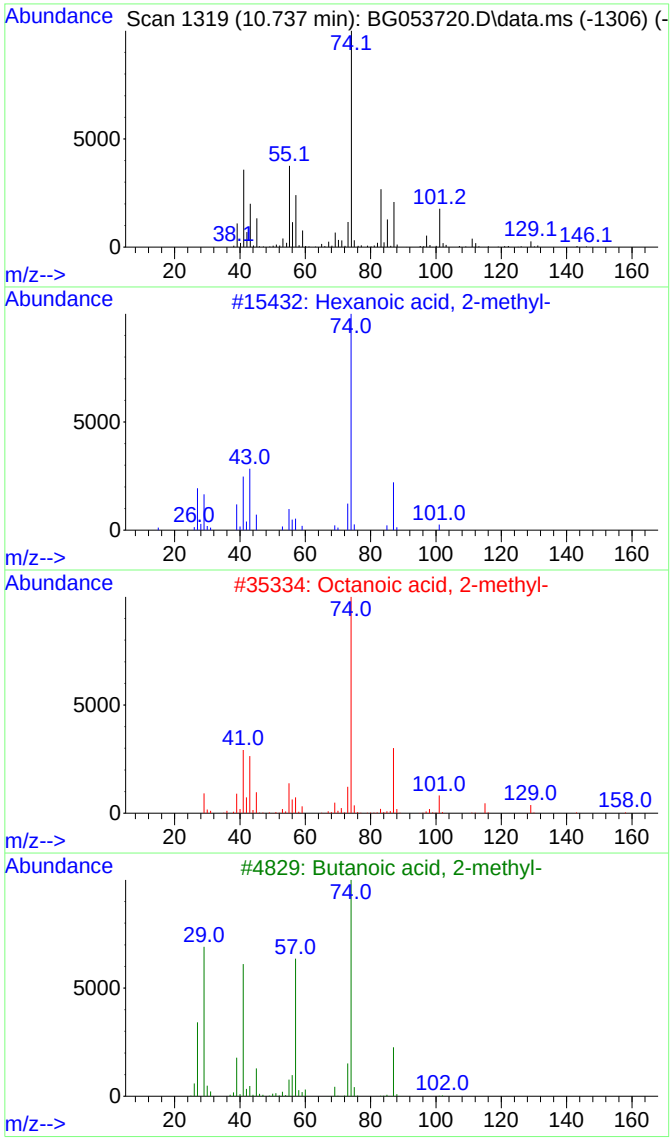
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

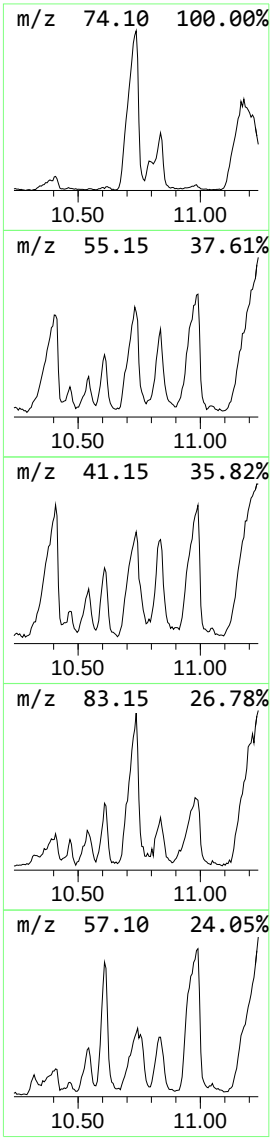
****

Peak Number 6 Hexanoic acid, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.737	61.75 ng	857206	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	53
2	Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	53
3	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	42
4	2,3-Dimethylpentanoic acid	130	C7H14O2	082608-03-5	40
5	Hexanoic acid, 5-methyl-, methyl...	144	C8H16O2	002177-83-5	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

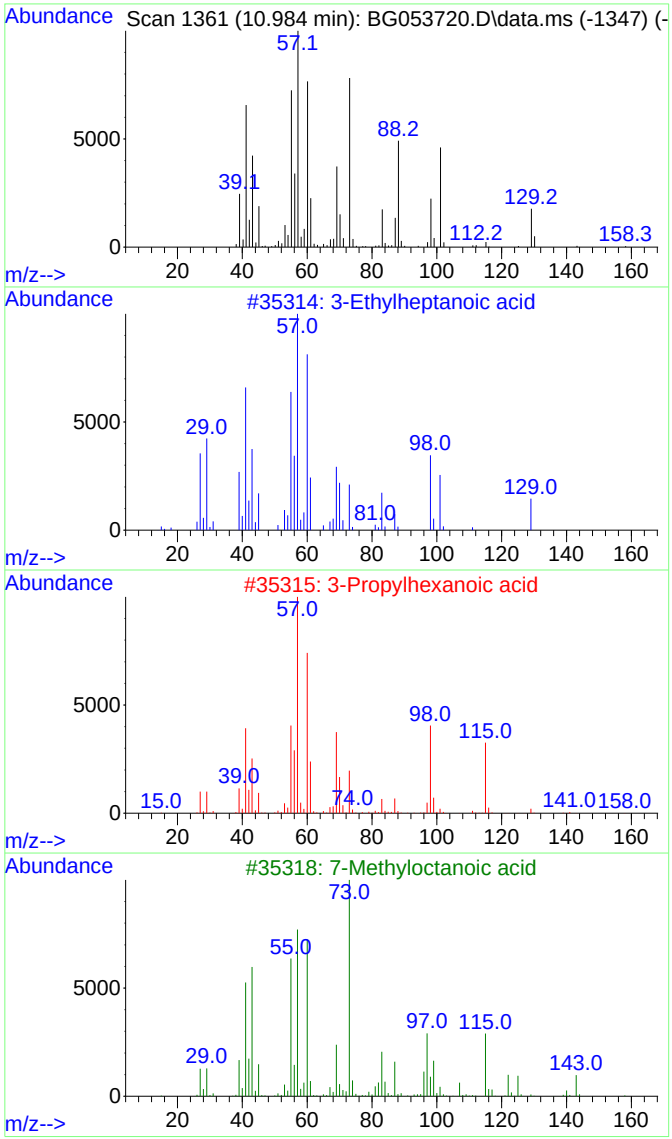
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

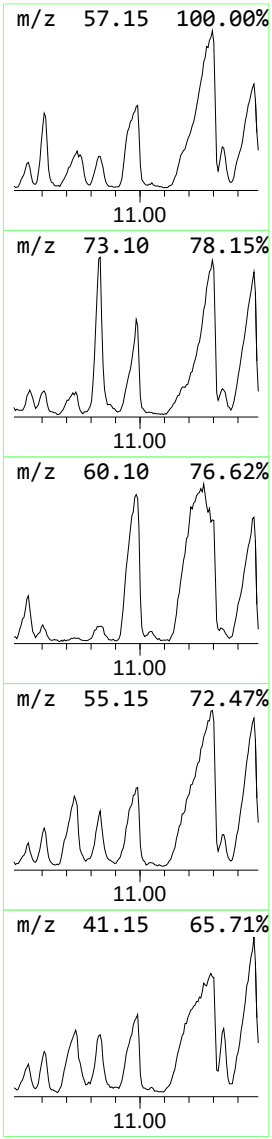
****

Peak Number 7 unknown10.984 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.984	73.59 ng	1021560	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	40
2	3-Propylhexanoic acid	158	C9H18O2	025110-61-6	38
3	7-Methyloctanoic acid	158	C9H18O2	000693-19-6	35
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	35
5	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	27





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Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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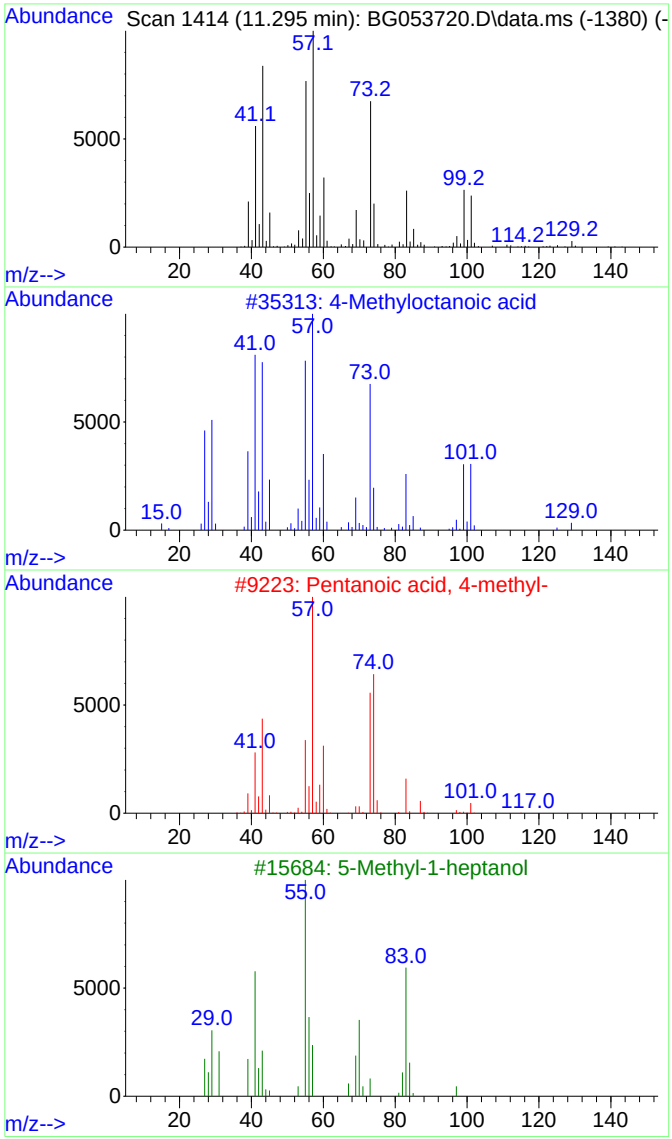
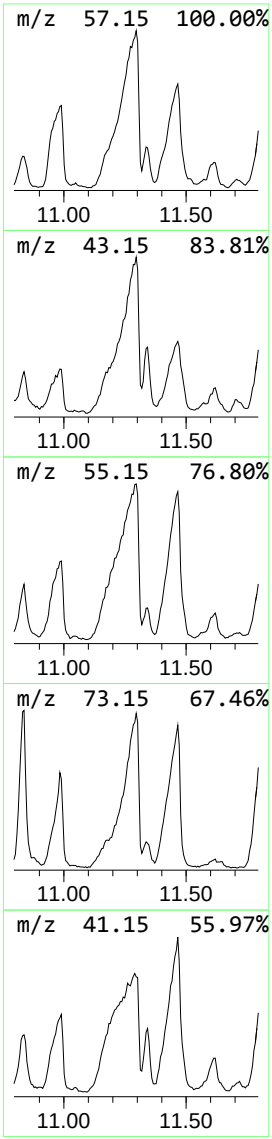
Peak Number 8 4-Methyloctanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.295	261.55 ng	3630640	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyloctanoic acid	158	C9H18O2	054947-74-9	80
2	Pentanoic acid, 4-methyl-	116	C6H12O2	000646-07-1	53
3	5-Methyl-1-heptanol	130	C8H18O	007212-53-5	22
4	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	22
5	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	16





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Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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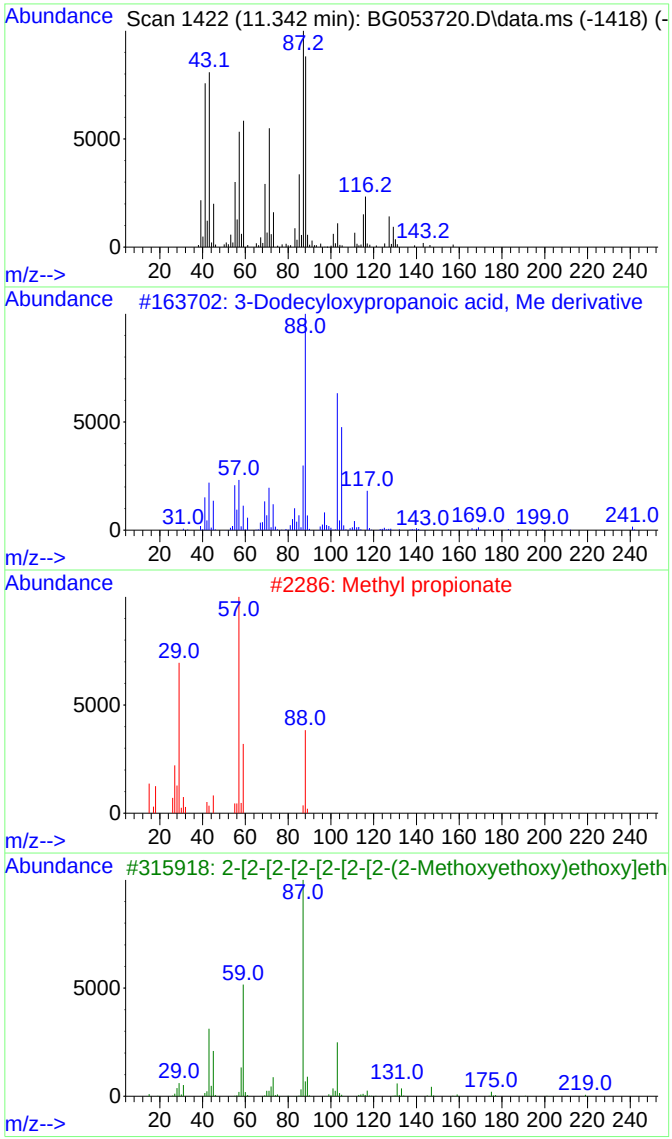
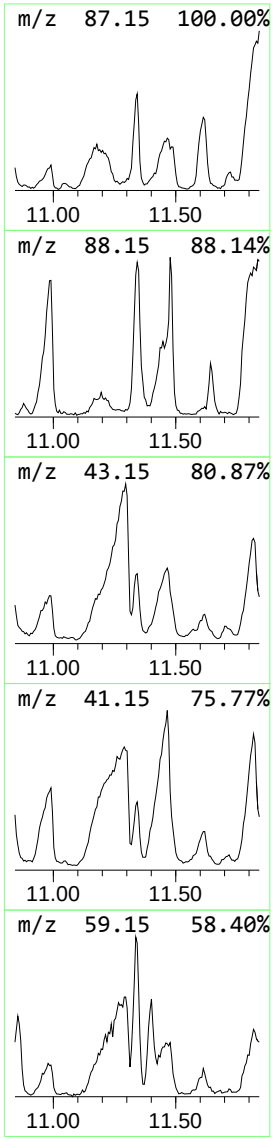
Peak Number 9 unknown11.342 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.342	26.11 ng	362470	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Dodecyloxypropanoic acid, Me d...	272	C16H32O3	1000497-89-8	35
2	Methyl propionate	88	C4H8O2	000554-12-1	27
3	2-[2-[2-[2-[2-[2-(2-Methoxyet...	426	C19H38O10	1000351-91-7	27
4	Ethyl 4-acetoxybutanoate	174	C8H14O4	025560-91-2	27
5	2-[2-[2-[2-[2-[2-(2-Methoxyethox...	382	C17H34O9	1010351-91-6	27





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Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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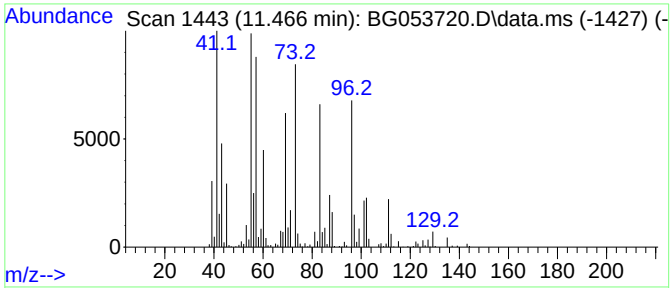
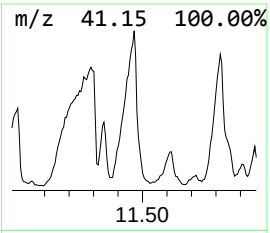
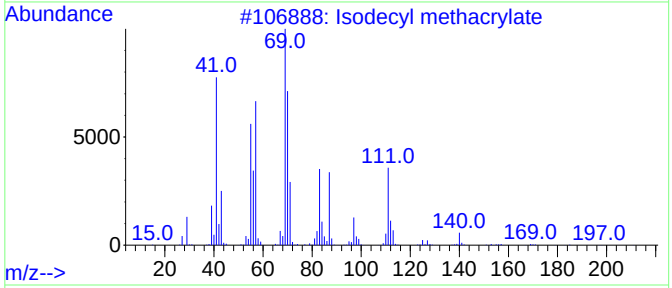
Peak Number 10 unknown11.466 Concentration Rank 3

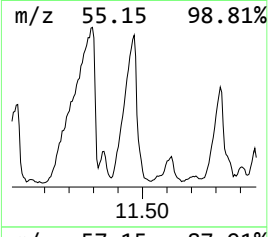
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.466	154.86 ng	2149670	Naphthalene-d8	10.796

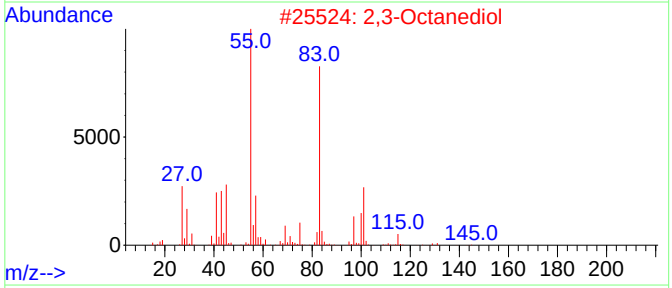
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isodecyl methacrylate	226	C14H26O2	029964-84-9	14
2	2,3-Octanediol	146	C8H18O2	020653-90-1	14
3	1-Isobutyl-1H-pyrazol-5-ylamine	139	C7H13N3	003524-18-3	12
4	3-Ethyl-4-methyl-2-pentene	112	C8H16	019780-68-8	11
5	3-Hexene, 2,4-dimethyl-	112	C8H16	082085-14-1	11

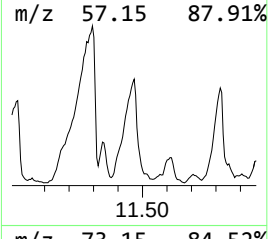


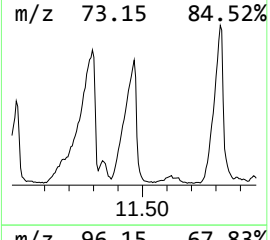


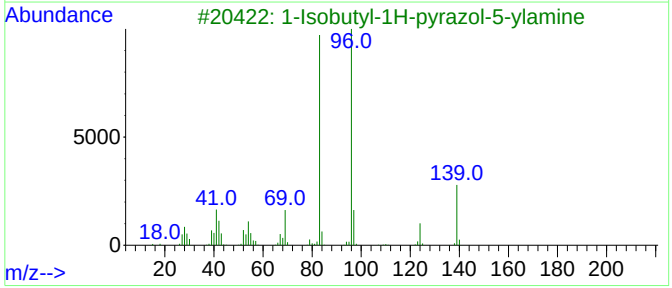


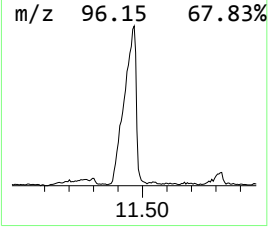












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Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

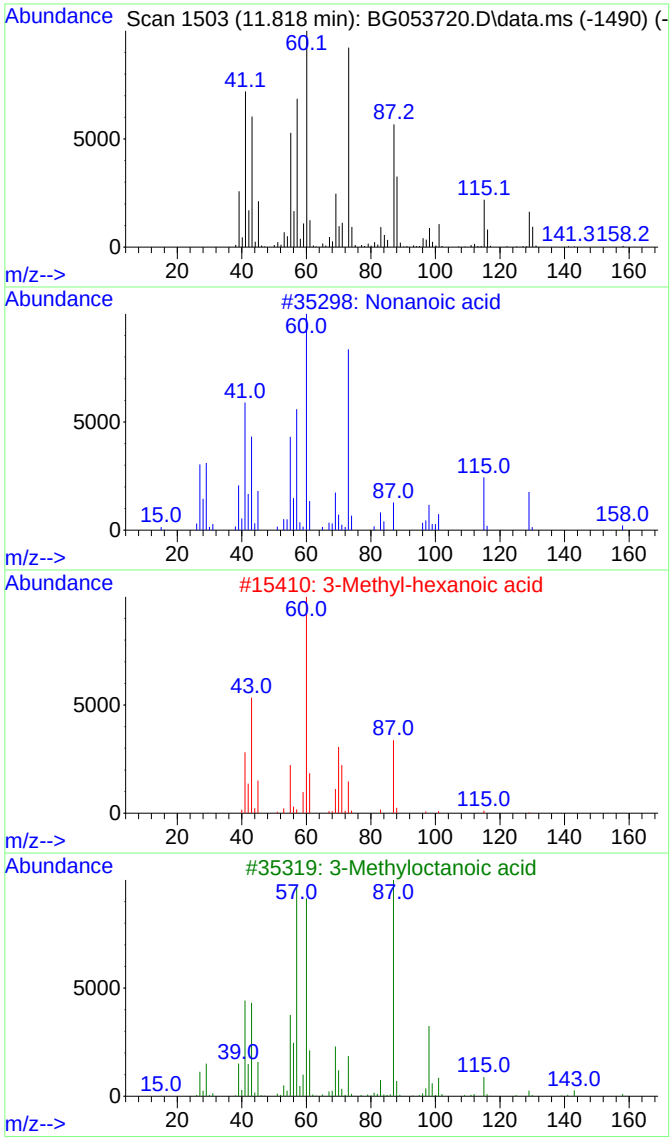
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

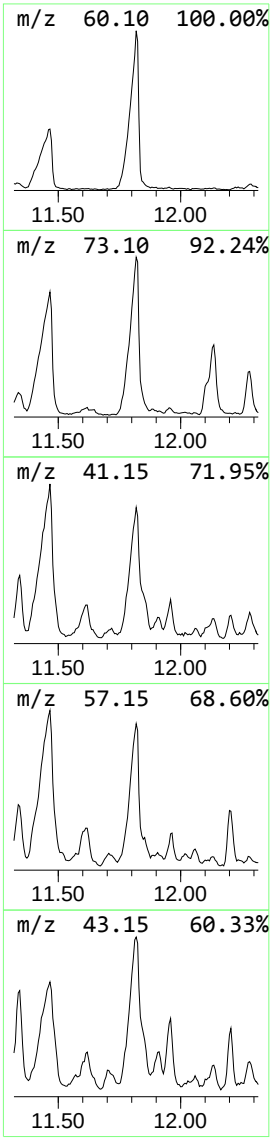
****

Peak Number 11 Nonanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.818	129.53 ng	1797950	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	58
2	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	50
3	3-Methyloctanoic acid	158	C9H18O2	006061-10-5	43
4	Hexanoic acid	116	C6H12O2	000142-62-1	43
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43





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Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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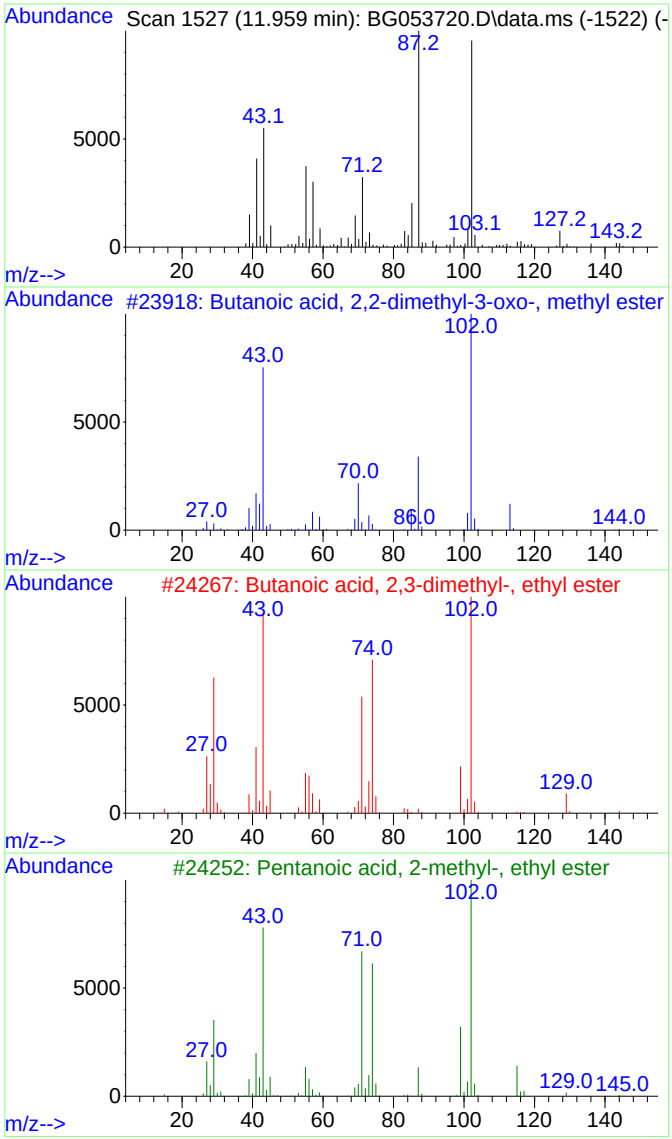
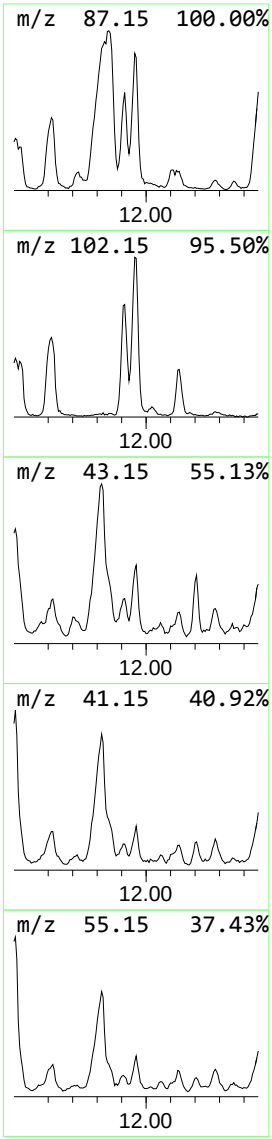
Peak Number 12 Butanoic acid, 2,2-dimethyl... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.959	25.87 ng	359090	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2,2-dimethyl-3-ox...	144	C7H12O3	038923-57-8	50
2	Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	38
3	Pentanoic acid, 2-methyl-, ethyl...	144	C8H16O2	039255-32-8	38
4	2-[2-(2-Butoxyethoxy)ethoxy]ethy...	248	C12H24O5	1000351-94-1	35
5	Bamifylline	385	C20H27N5O3	002016-63-9	27





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Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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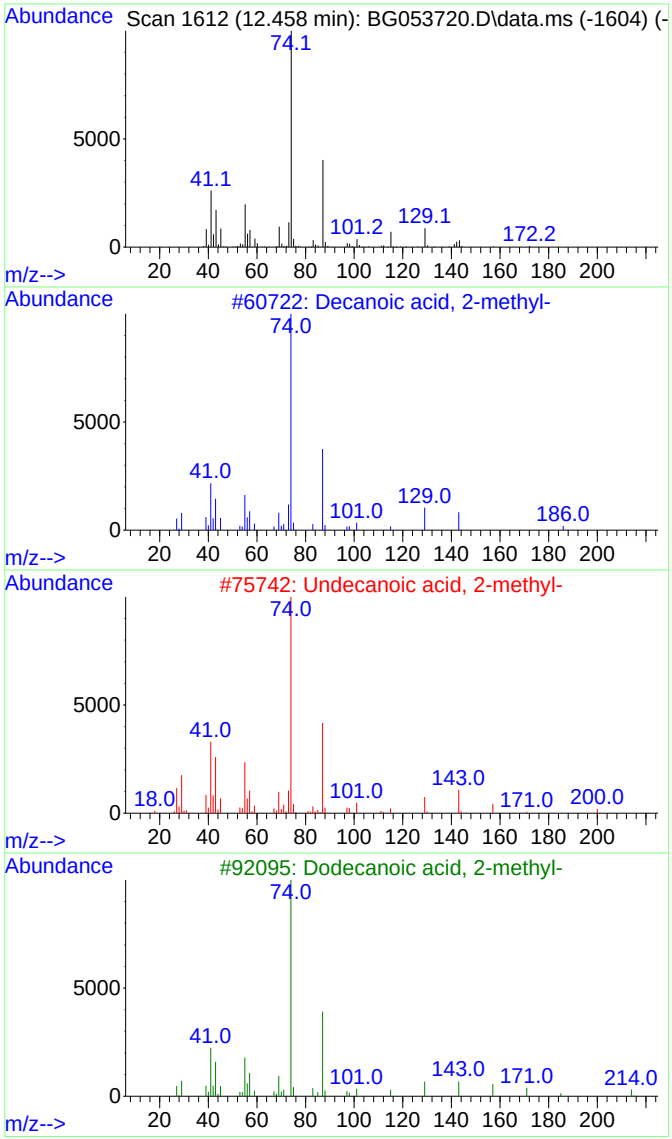
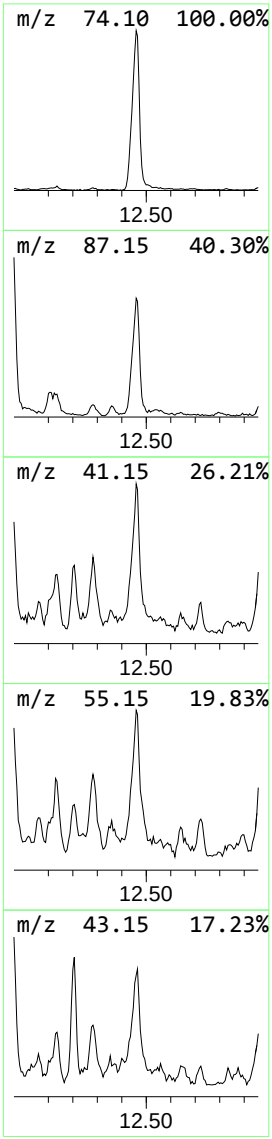
Peak Number 13 Decanoic acid, 2-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.459	34.48 ng	478586	Naphthalene-d8	10.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	90
2	Undecanoic acid, 2-methyl-	200	C12H24O2	024323-25-9	83
3	Dodecanoic acid, 2-methyl-	214	C13H26O2	002874-74-0	78
4	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	64
5	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64





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Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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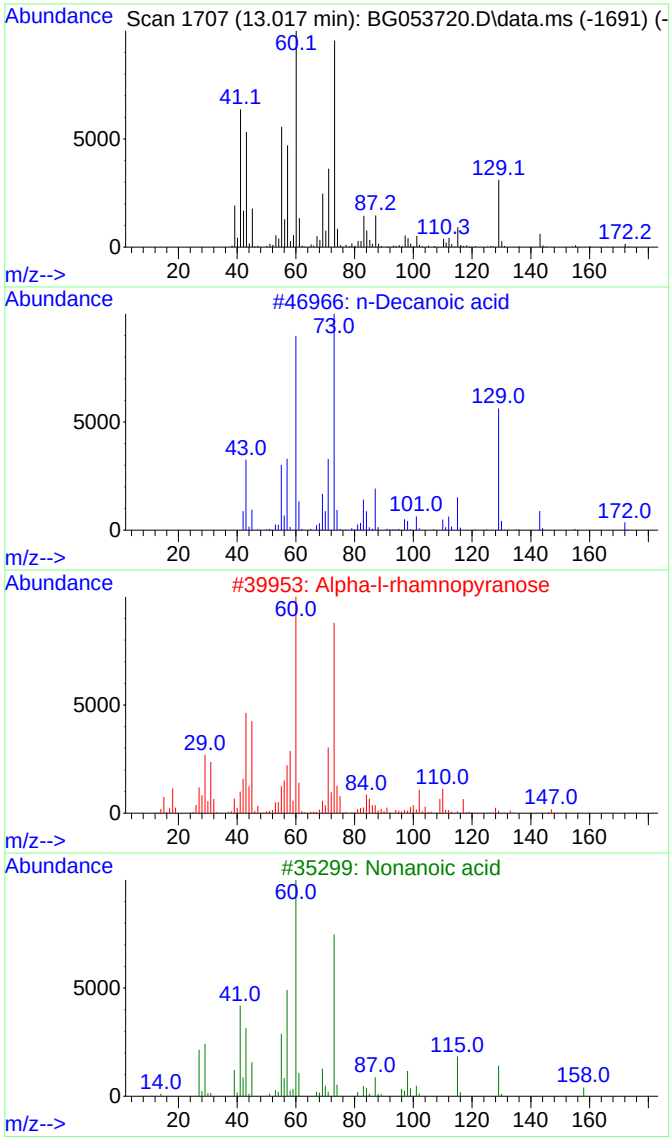
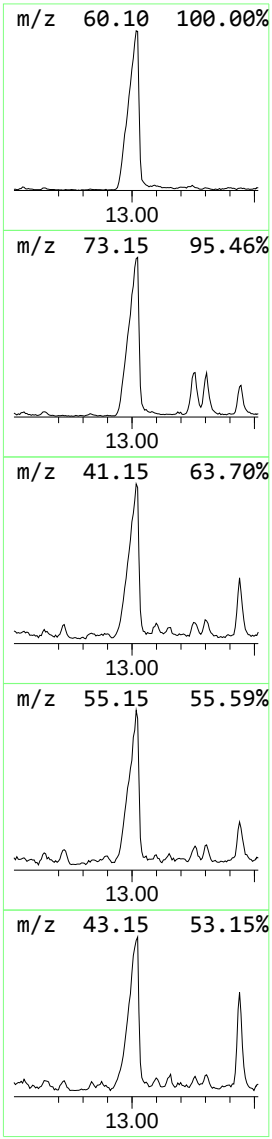
Peak Number 14 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.017	70.19 ng	1544960	Acenaphthene-d10	14.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	97
2	Alpha-l-rhamnopyranose	164	C6H12O5	035810-56-1	53
3	Nonanoic acid	158	C9H18O2	000112-05-0	53
4	Hexanoic acid	116	C6H12O2	000142-62-1	50
5	Octanoic acid	144	C8H16O2	000124-07-2	50





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Acq On : 26 May 2022 17:04
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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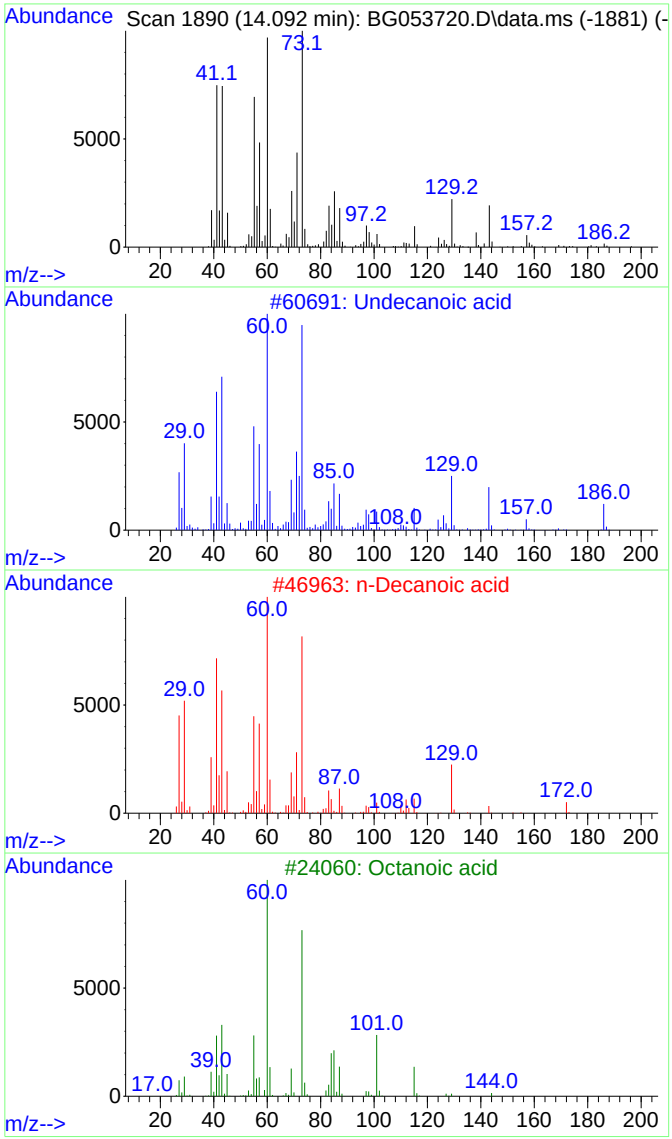
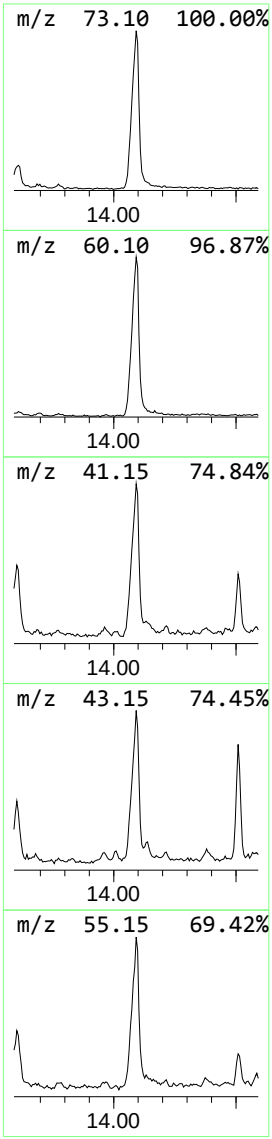
Peak Number 15 Undecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	38.15 ng	839689	Acenaphthene-d10	14.626

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	87
2	n-Decanoic acid	172	C10H20O2	000334-48-5	59
3	Octanoic acid	144	C8H16O2	000124-07-2	43
4	Heptanoic acid	130	C7H14O2	000111-14-8	35
5	Hexanoic acid	116	C6H12O2	000142-62-1	27





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ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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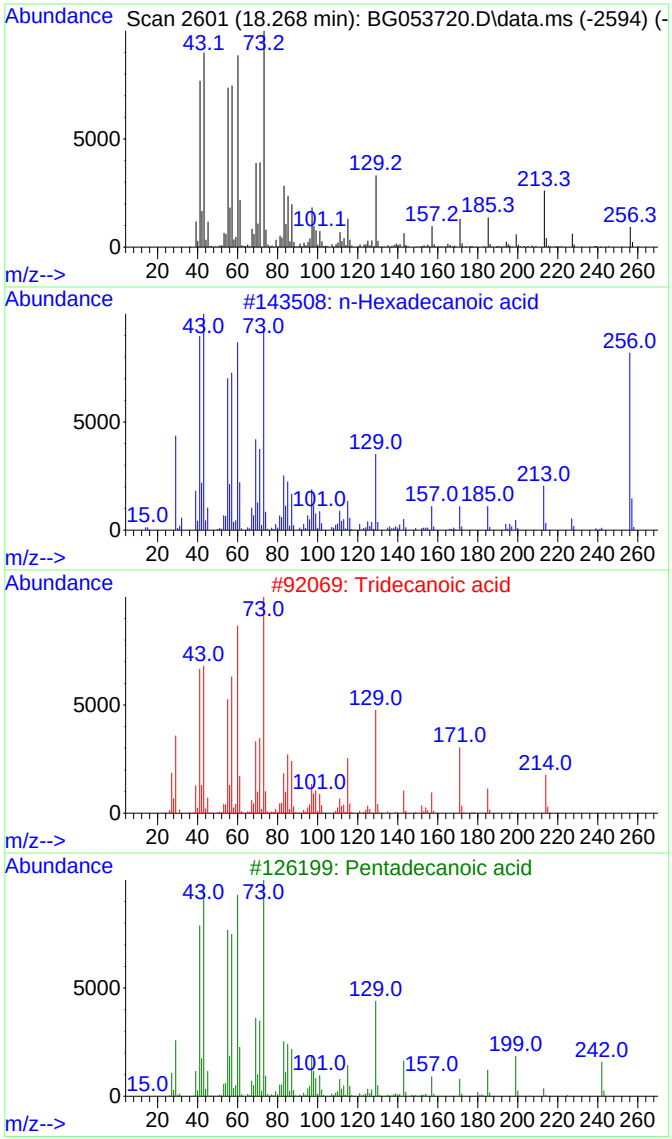
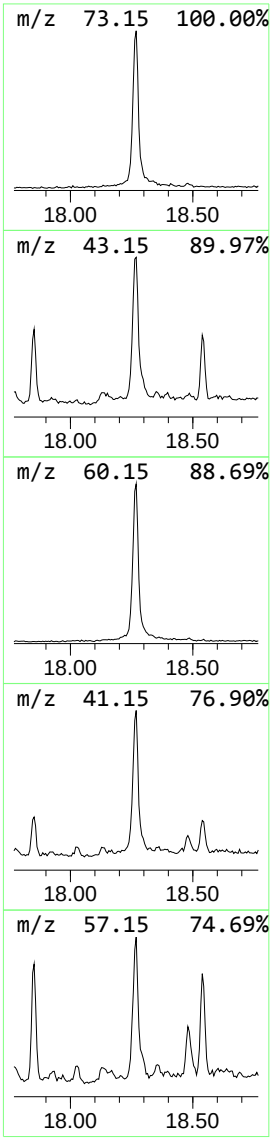
Peak Number 16 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	55.24 ng	1046300	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





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Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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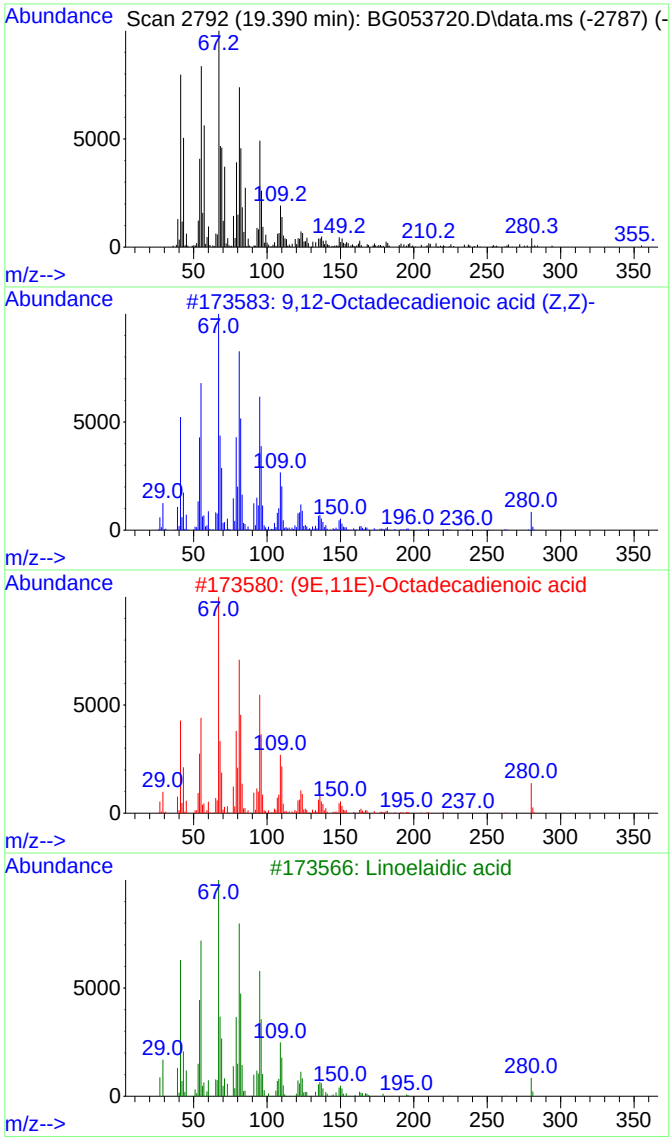
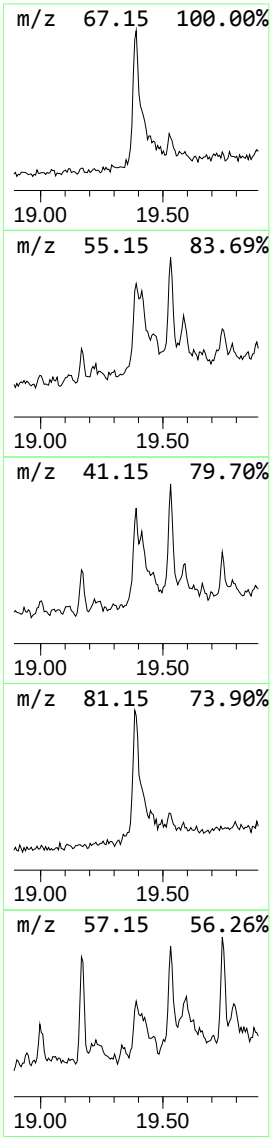
Peak Number 17 9,12-Octadecadienoic acid (... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.390	26.38 ng	499625	Phenanthrene-d10	17.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	96
3	Linoelaidic acid	280	C18H32O2	000506-21-8	96
4	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	96
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	89





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Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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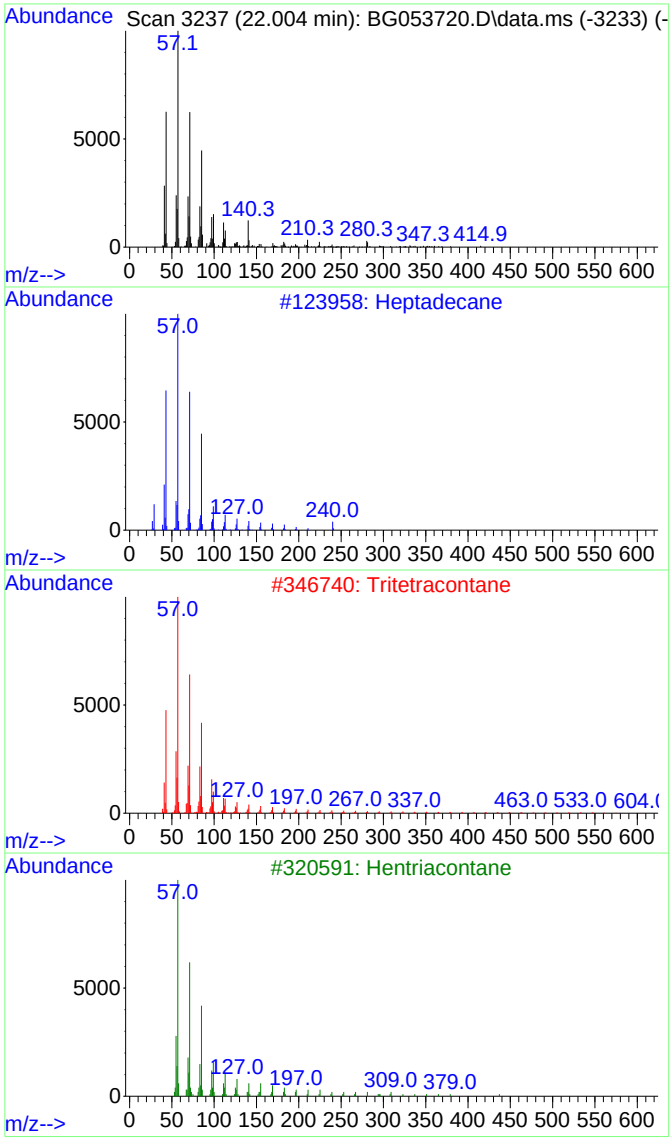
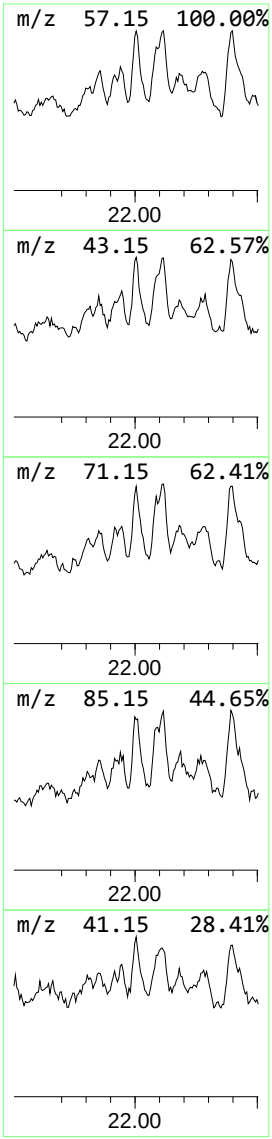
Peak Number 18 Heptadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.004	25.81 ng	561768	Chrysene-d12	21.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tritetracontane	605	C43H88	007098-21-7	90
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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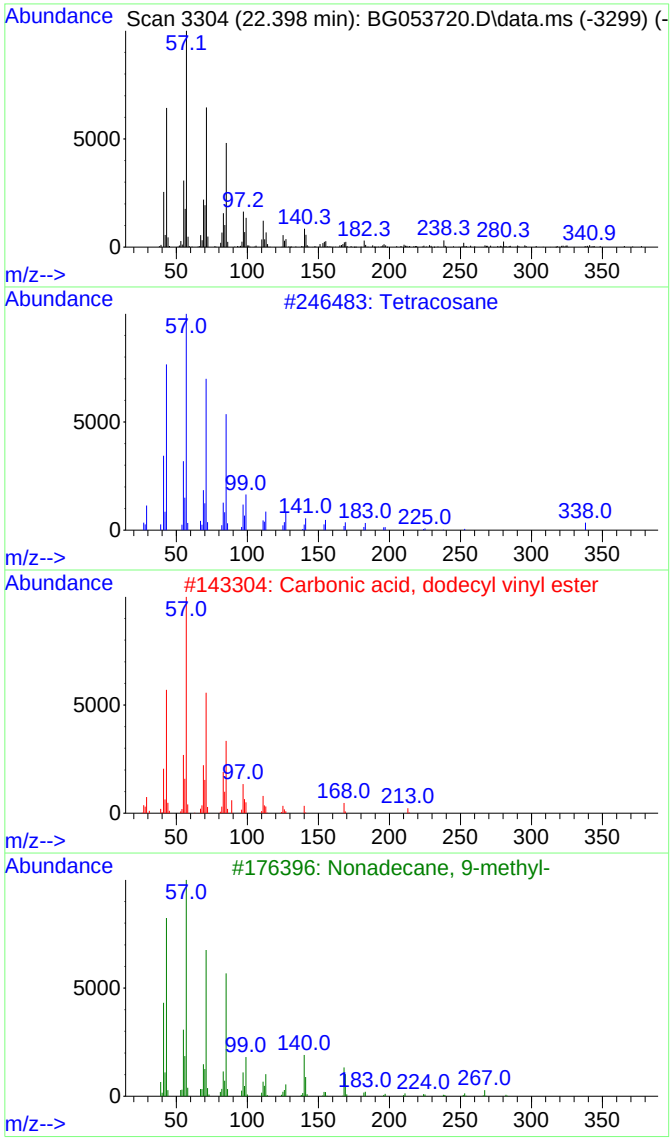
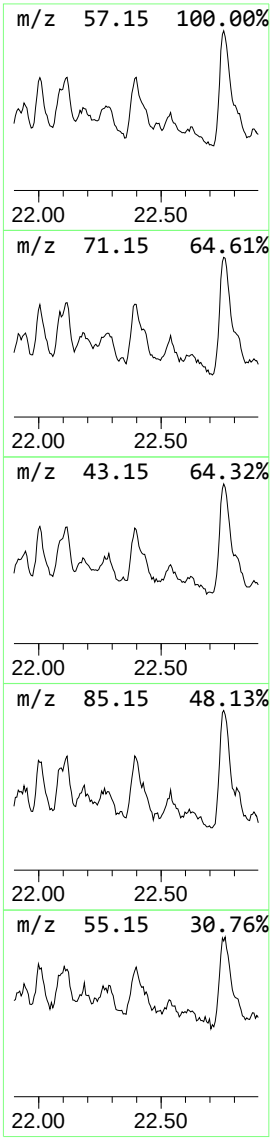
Peak Number 19 Tetracosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.398	35.97 ng	782803	Chrysene-d12	21.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	86
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
4	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	80
5	Nonadecane	268	C19H40	000629-92-5	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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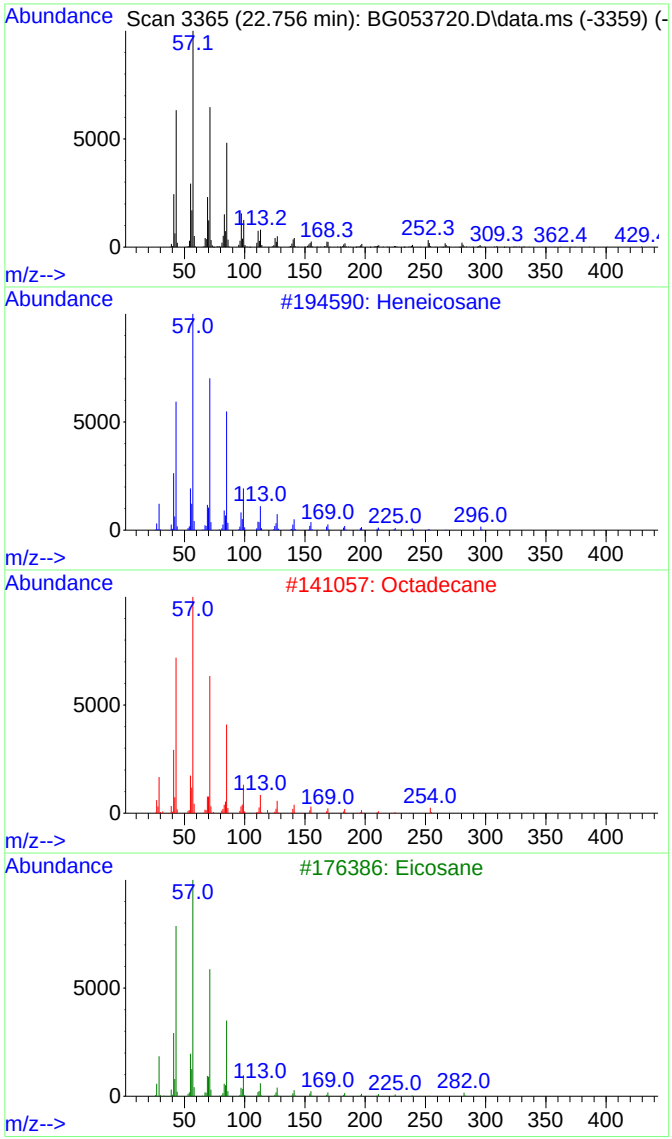
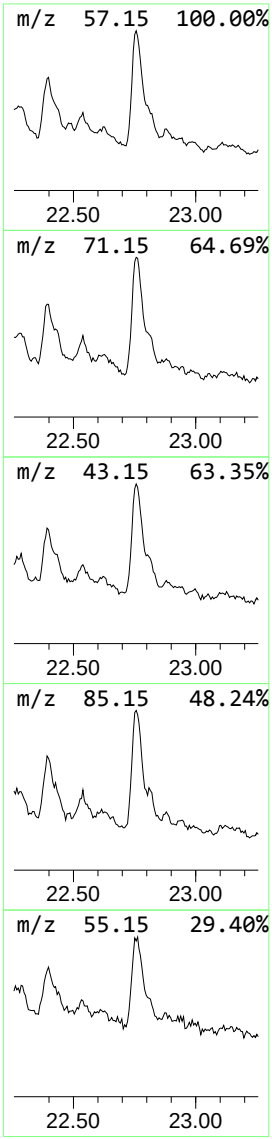
Peak Number 20 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.756	86.78 ng	1888700	Chrysene-d12	21.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Octadecane	254	C18H38	000593-45-3	94
3	Eicosane	282	C20H42	000112-95-8	93
4	Tricosane	324	C23H48	000638-67-5	91
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052622\
Data File : BG053720.D
Acq On : 26 May 2022 17:04
Operator : CG/JU
Sample : N3059-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
4922A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.095	68.1	ng	1062460	1	7.982	312071	20.0
Hexanoic acid, ...	9.733	633.2	ng	8789000	2	10.796	277620	20.0
unknown9.956	9.956	113.9	ng	1580560	2	10.796	277620	20.0
unknown10.109	10.109	92.2	ng	1279130	2	10.796	277620	20.0
Octanoic acid	10.408	88.2	ng	1223910	2	10.796	277620	20.0
Hexanoic acid, ...	10.737	61.8	ng	857206	2	10.796	277620	20.0
unknown10.984	10.984	73.6	ng	1021560	2	10.796	277620	20.0
4-Methyloctanoi...	11.295	261.6	ng	3630640	2	10.796	277620	20.0
unknown11.342	11.342	26.1	ng	362470	2	10.796	277620	20.0
unknown11.466	11.466	154.9	ng	2149670	2	10.796	277620	20.0
Nonanoic acid	11.818	129.5	ng	1797950	2	10.796	277620	20.0
Butanoic acid, ...	11.959	25.9	ng	359090	2	10.796	277620	20.0
Decanoic acid, ...	12.459	34.5	ng	478586	2	10.796	277620	20.0
n-Decanoic acid	13.017	70.2	ng	1544960	3	14.626	440205	20.0
Undecanoic acid	14.092	38.1	ng	839689	3	14.626	440205	20.0
n-Hexadecanoic ...	18.268	55.2	ng	1046300	4	17.369	378831	20.0
9,12-Octadecadi...	19.390	26.4	ng	499625	4	17.369	378831	20.0
Heptadecane	22.004	25.8	ng	561768	5	21.634	435307	20.0
Tetracosane	22.398	36.0	ng	782803	5	21.634	435307	20.0
Heneicosane	22.756	86.8	ng	1888700	5	21.634	435307	20.0