LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-29

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_F\Methods\8270-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.234	154	161	167	rBV	35631	59203	1.78%	0.218%
2	3.393	182	188	201	rVB	92360	166141	4.99%	0.612%
3	3.863	256	268	276	rVB	51531	90113	2.70%	0.332%
4	3.975	282	287	293	rBV	61318	79741	2.39%	0.294%
5	5.110	476	480	482	rBV	32665	41397	1.24%	0.153%
6	5.187	482	493	499	rVB3	40349	118738	3.56%	0.438%
7	5.375	521	525	529	rVB	782782	677284	20.33%	2.496%
8	5.510	539	548	552	rBV2	1535546	1821310	54.67%	6.712%
9	5.616	555	566	568	rBV	28057	51403	1.54%	0.189%
10	5.687	575	578	583	rBV	47218	42722	1.28%	0.157%
11	5.740	583	587	590	rBV	584140	499874	15.00%	1.842%
12	5.998	625	631	638	rBV	55916	110366	3.31%	0.407%
13	6.057	638	641	644	rVB	81154	63802	1.92%	0.235%
14	6.345	688	690	694	rBV	78747	63174	1.90%	0.233%
15	6.410	699	701	704	rVV	69142	51946	1.56%	0.191%
16	6.445	704	707	710	rVV	164087	135001	4.05%	0.497%
17	6.487	710	714	716	rVV2	64205	57081	1.71%	0.210%
18	6.516	716	719	724	rVV	854422	846819	25.42%	3.121%
19	6.575	726	729	732	rVB	190592	164965	4.95%	0.608%
20	6.710	749	752	758	rVB	692578	554801	16.65%	2.045%
21	6.887	779	782	785	rBV	613957	525171	15.76%	1.935%
22	6.945	789	792	797	rVB	403278	351540	10.55%	1.295%
23	7.069	809	813	816	rBV	261689	224128	6.73%	0.826%
24	7.145	822	826	833	rBV5	34300	71146	2.14%	0.262%
25	7.204	833	836	841	rBV3	49883	65231	1.96%	0.240%
26	7.292	846	851	854	rBV3	106261	124445	3.74%	0.459%
27	7.422	867	873	875	rBV3	139261	204851	6.15%	0.755%
28	7.457	875	879	882	rVV	2252598	2121684	63.69%	7.819%
29	7.510	885	888	893	rVV2	44088	59582	1.79%	0.220%
30	7.563	893	897	901	rVB3	67422	88691	2.66%	0.327%
31	7.657	910	913	915	rBV	59588	54182	1.63%	0.200%
32	7.681	915	917	922	rVV3	83109	134874	4.05%	0.497%
33	7.739	922	927	930	rVB3	60413	79840	2.40%	0.294%
34	7.839	942	944	949	rVB2	52410	57187	1.72%	0.211%
35	7.910	949	956	962	rBV3	216011	436246	13.09%	1.608%
36	8.010	970	973	981	rVB5	41761	73946	2.22%	0.273%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

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_F\Methods\8270-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.075	981	984	989	rBV	134261	158250	4.75%	0.583%
38	8.175	997	1001	1003	rBV	832942	715226	21.47%	2.636%
39	8.192	1003	1004	1007	rVB	260293	172486	5.18%	0.636%
40	8.434	1039	1045	1046	rBV2	178734	218174	6.55%	0.804%
41	8.451	1046	1048	1053	rVB	337923	295568	8.87%	1.089%
42	8.545	1058	1064	1067	rVV6	73260	125552	3.77%	0.463%
43	8.604	1067	1074	1078	rBV2	290671	366725	11.01%	1.351%
44	8.763	1096	1101	1105	rBV5	49063	69795	2.09%	0.257%
45	8.886	1118	1122	1124	rBV3	55582	68897	2.07%	0.254%
46	8.933	1128	1130	1133	rVV2	83699	76856	2.31%	0.283%
47	8.986	1136	1139	1141	rVV	229054	209257	6.28%	0.771%
48	9.010	1141	1143	1146	rVV2	118107	126160	3.79%	0.465%
49	9.045	1146	1149	1154	rVB3	73328	86558	2.60%	0.319%
50	9.175	1165	1171	1176	rBV5	166252	288018	8.65%	1.061%
51	9.251	1179	1184	1187	rVB	4095376	3331504	100.00%	12.277%
52	9.322	1193	1196	1198	rBV	95674	80388	2.41%	0.296%
53	9.439	1213	1216	1220	rVB2	96366	102309	3.07%	0.377%
54	9.498	1223	1226	1228	rVV3	49300	42948	1.29%	0.158%
55	9.686	1253	1258	1263	rBV	382217	409089	12.28%	1.508%
56	9.739	1263	1267	1272	rVB4	86688	141801	4.26%	0.523%
57	9.792	1272	1276	1278	rBV	125527	116161	3.49%	0.428%
58	9.851	1278	1286	1289	rBV	488894	688057	20.65%	2.536%
59	9.886	1289	1292	1294	rVB2	116749	104788	3.15%	0.386%
60	9.933	1296	1300	1303	rVB	923523	731054	21.94%	2.694%
61	10.092	1324	1327	1332	rBV6	57497	89998	2.70%	0.332%
62	10.351	1369	1371	1374	rVB2	105771	81106	2.43%	0.299%
63	10.569	1405	1408	1410	rVB2	51252	49048	1.47%	0.181%
64	10.727	1430	1435	1438	rBV	2588002	2213955	66.46%	8.159%
65	10.833	1449	1453	1460	rVB2	175049	257574	7.73%	0.949%
66	11.045	1486	1489	1494	rBV	127297	142630	4.28%	0.526%
67	11.274	1525	1528	1530	rBV	118484	97492	2.93%	0.359%
68	11.310	1530	1534	1538	rVB2	90814	103753	3.11%	0.382%
69	11.369	1541	1544	1546	rVB3	46870	40605	1.22%	0.150%
70	11.422	1550	1553	1556	rVB	790172	658207	19.76%	2.426%
71	11.580	1577	1580	1581	rBV	70921	60651	1.82%	0.224%
72	11.604	1581	1584	1587	rVB	177628	166552	5.00%	0.614%
73	11.698	1598	1600	1603	rVB	104798	92576	2.78%	0.341%
74	11.939	1638	1641	1645	rBV3	88816	96609	2.90%	0.356%
75	11.980	1645	1648	1650	rVV	63955	53836	1.62%	0.198%
76	12.110	1667	1670	1674	rVB	113168	90874	2.73%	0.335%

LSC Area Percent Report

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Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

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_F\Methods\8270-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	12.498	1734	1736	1739	rVB	89017	67193	2.02%	0.248%
78	12.869	1797	1799	1802	rBV	54524	50518	1.52%	0.186%
79	13.010	1819	1823	1826	rBV	2710156	2427226	72.86%	8.945%
80	13.227	1857	1860	1864	rBV	56565	59713	1.79%	0.220%
81	13.563	1914	1917	1921	rBV3	97743	116527	3.50%	0.429%
82	13.904	1972	1975	1982	rVB2	79735	111976	3.36%	0.413%
83	14.068	1999	2003	2006	rBV	464481	378791	11.37%	1.396%
84	14.215	2026	2028	2035	rVB3	40630	58769	1.76%	0.217%
85	15.562	2252	2257	2264	rVB	377172	475514	14.27%	1.752%

Sum of corrected areas: 27135939

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
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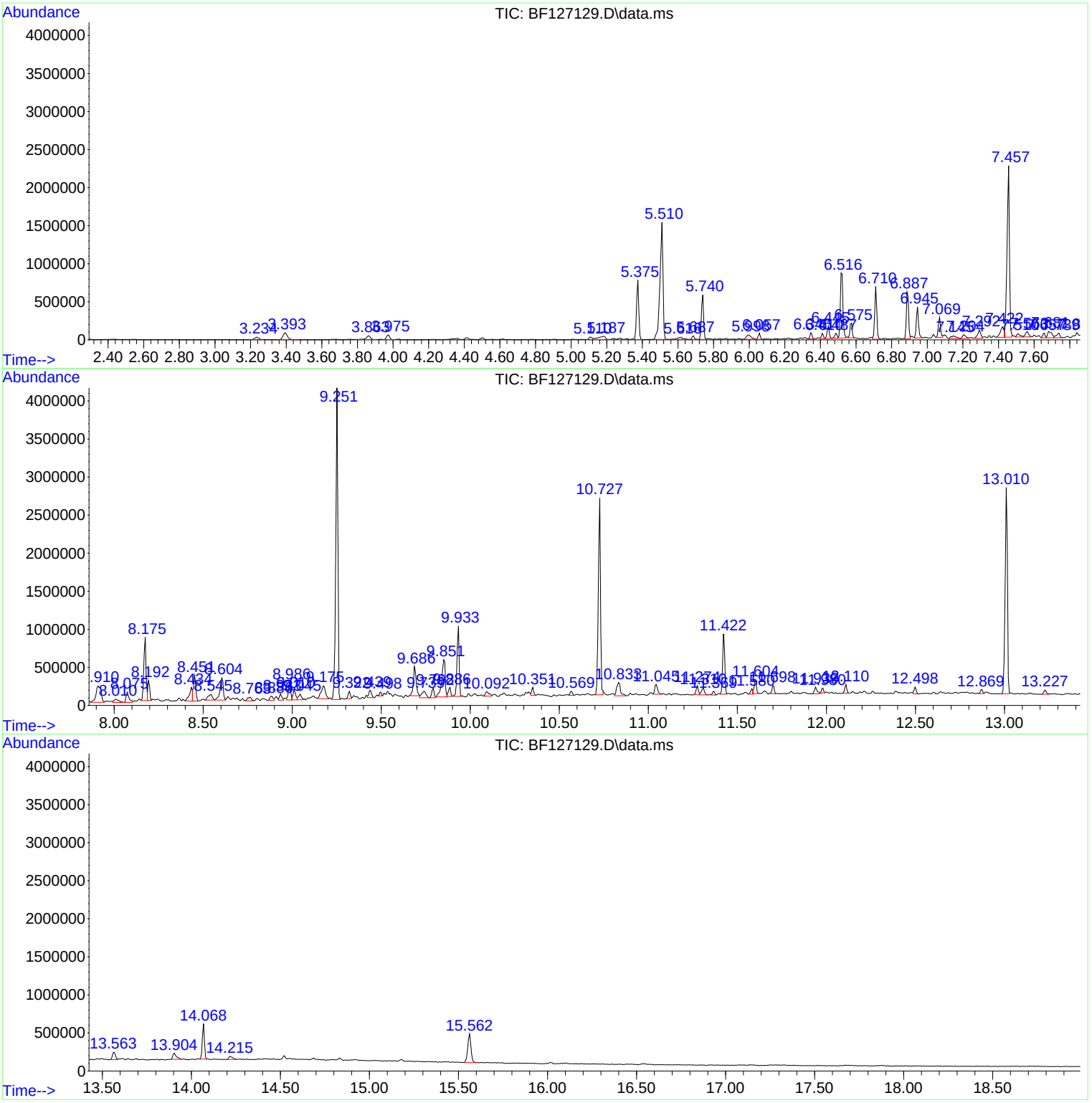
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

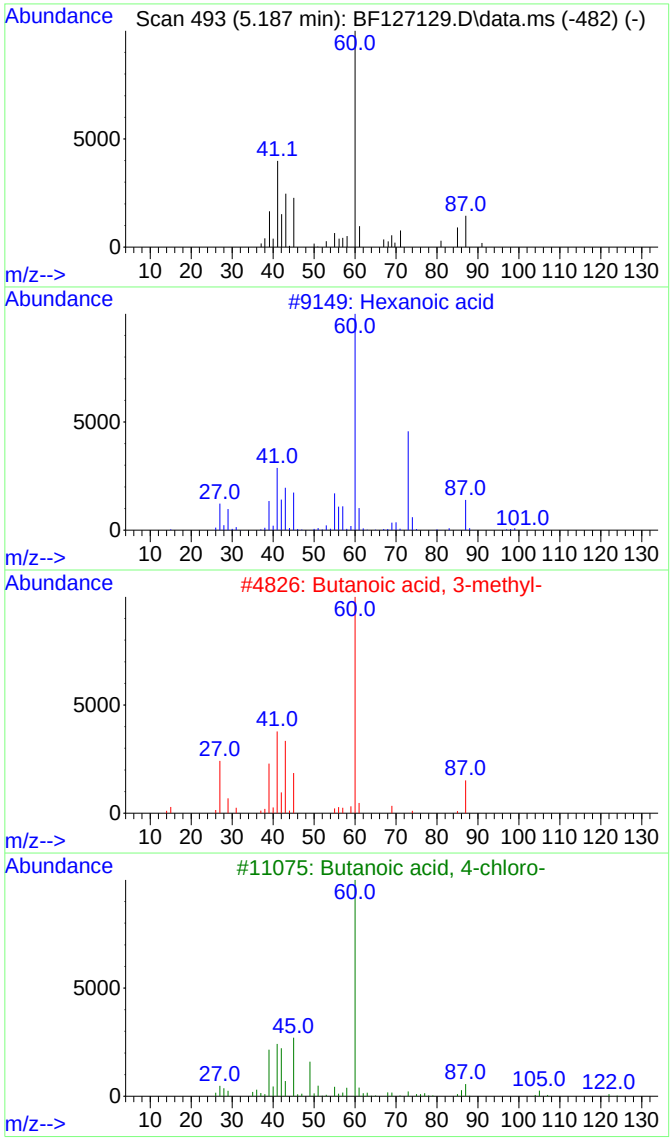
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

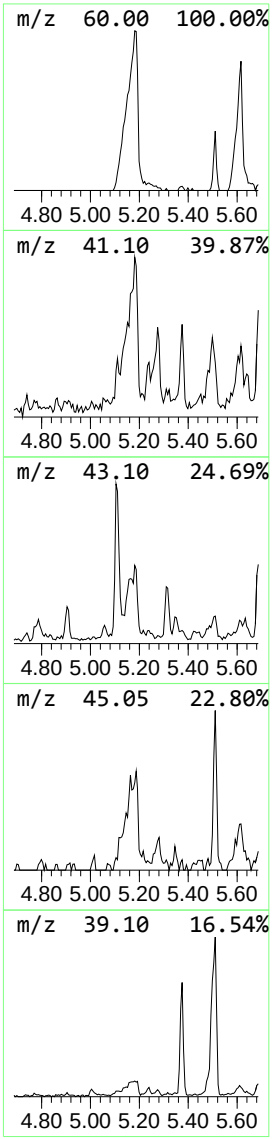
****

Peak Number 2 Hexanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	4.52 ng	118738	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	72
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
3	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	38
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	38
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

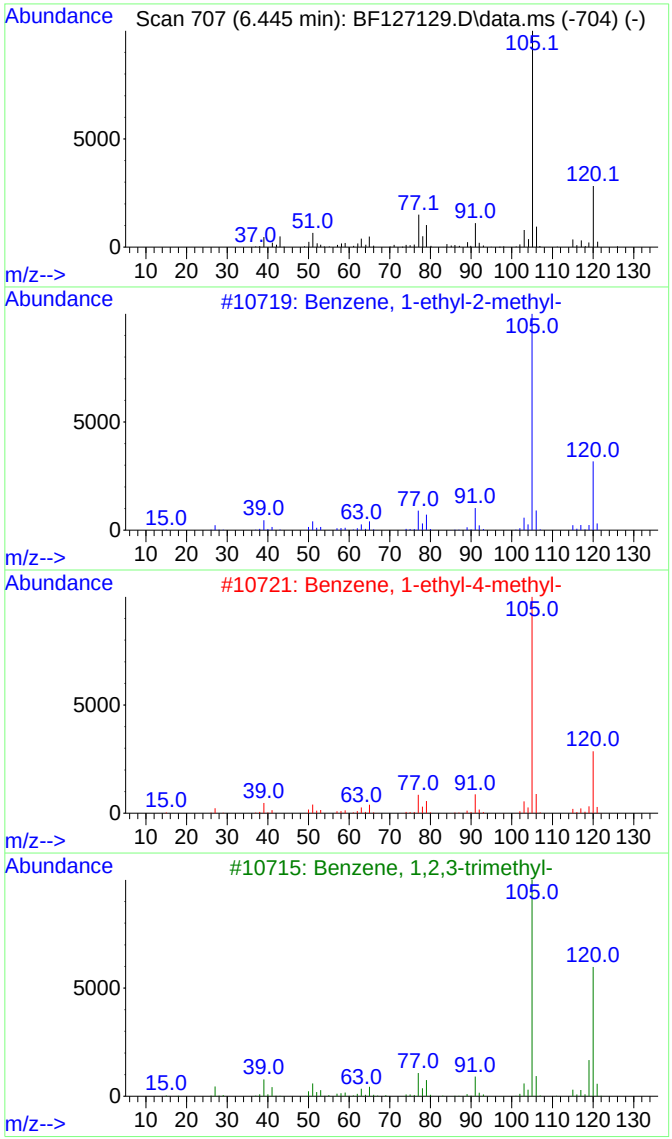
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

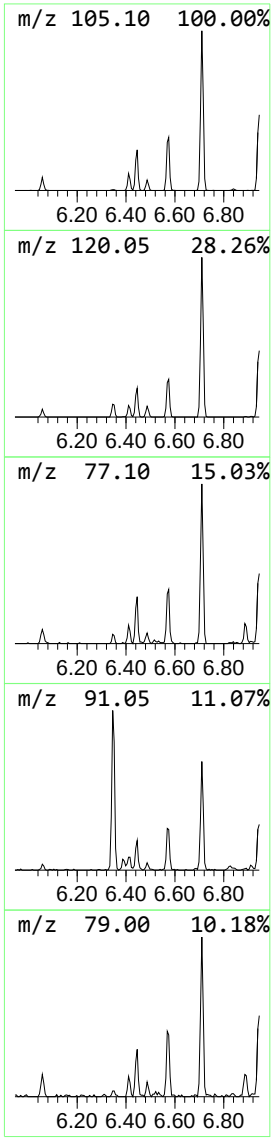
****

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.445	5.14 ng	135001	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

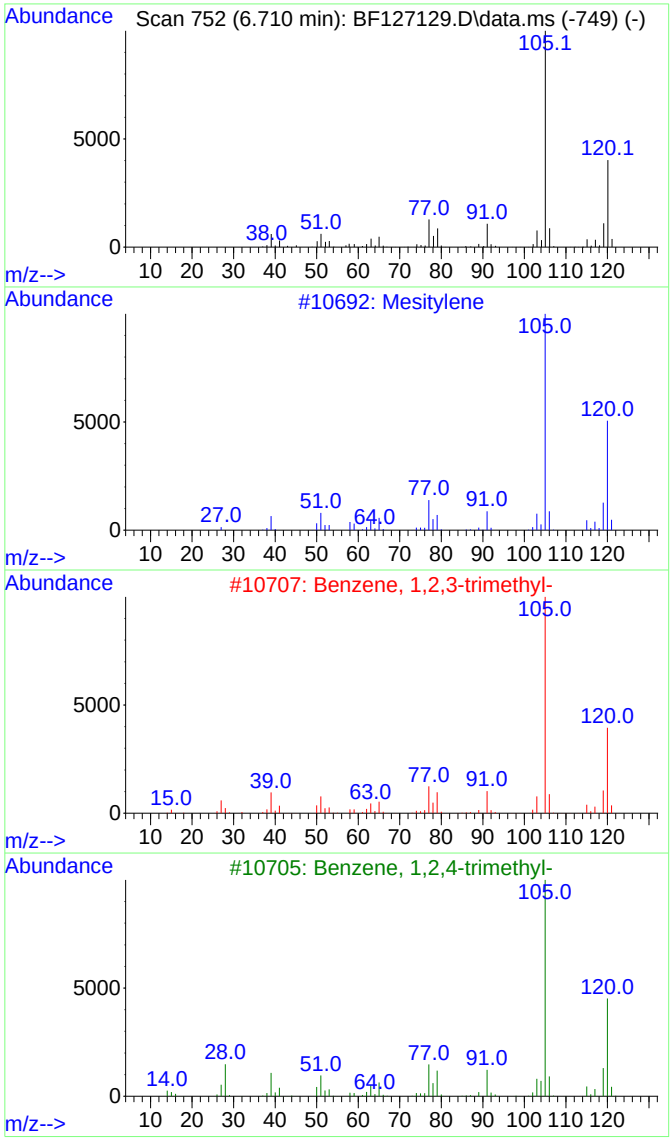
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

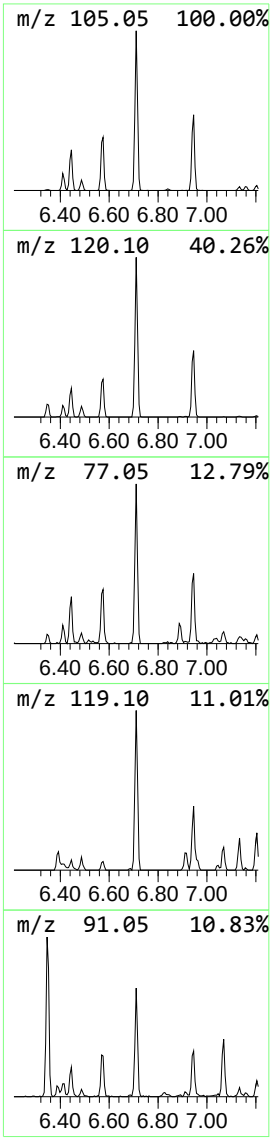
****

Peak Number 6 Mesitylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	21.13 ng	554801	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

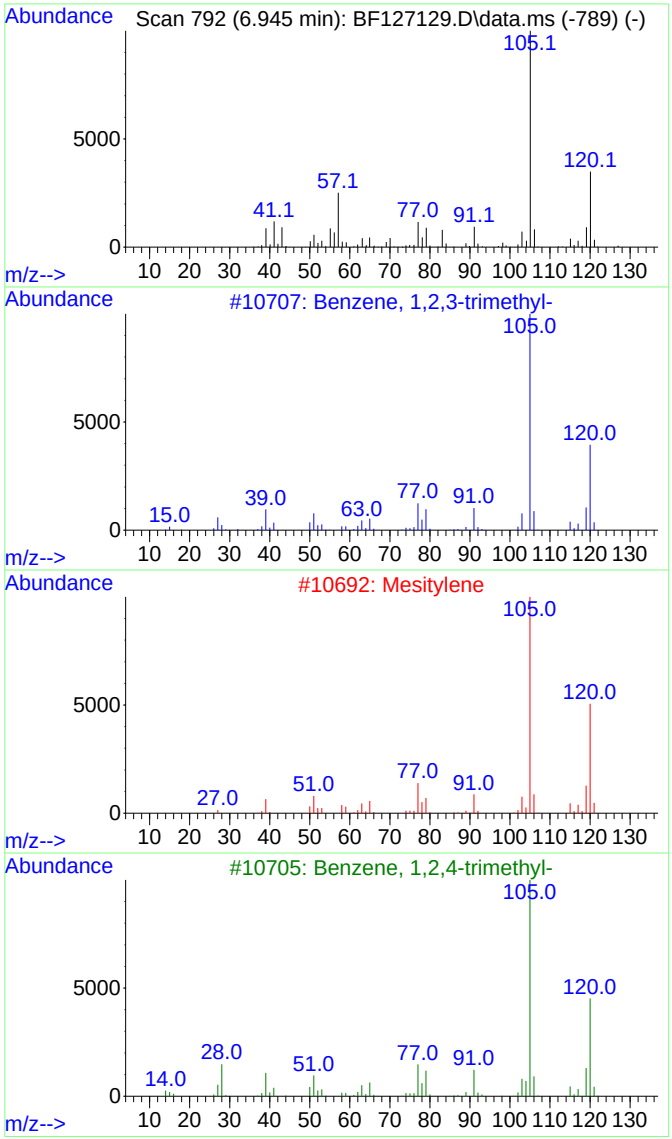
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

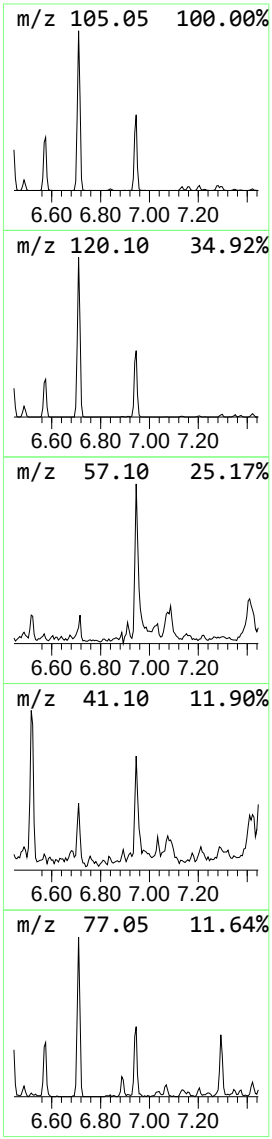
****

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.945	13.39 ng	351540	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

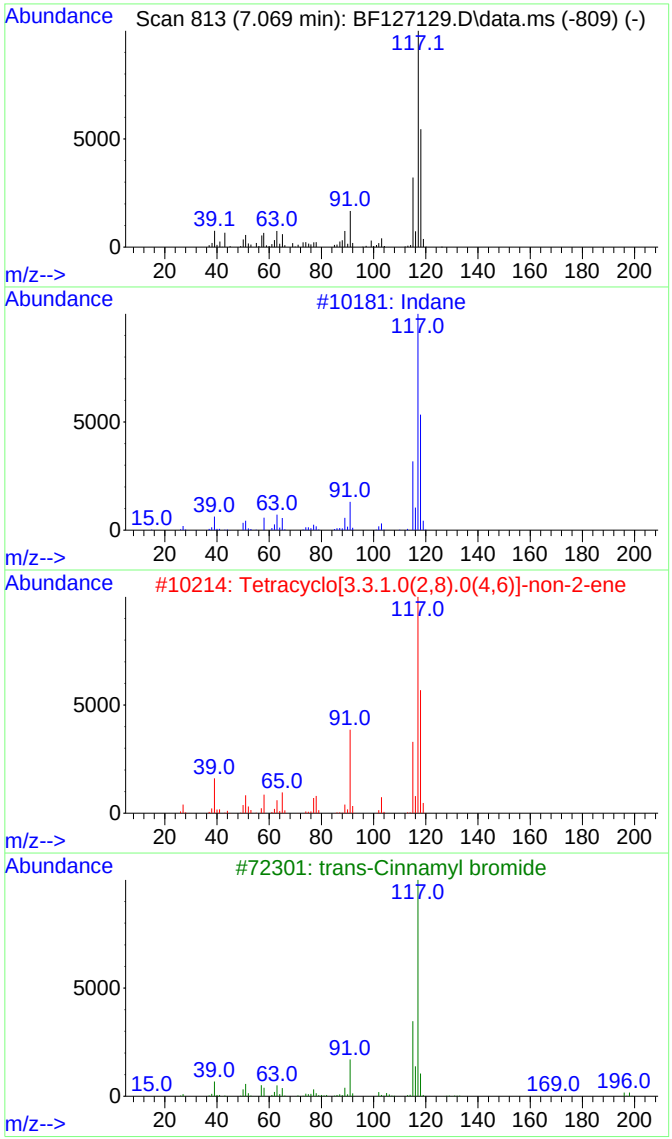
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

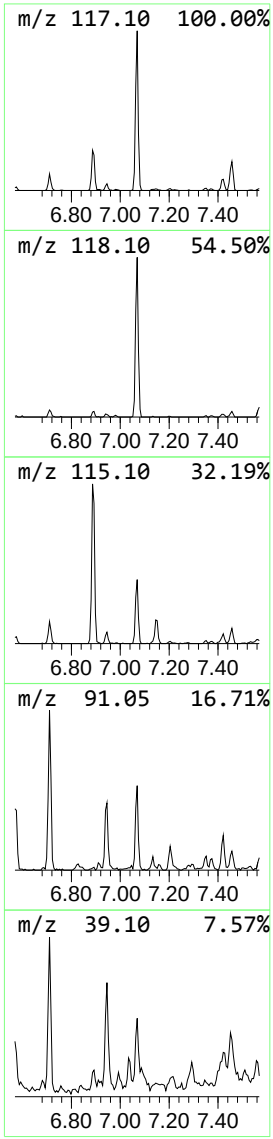
****

Peak Number 8 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	8.54 ng	224128	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
3	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
4	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

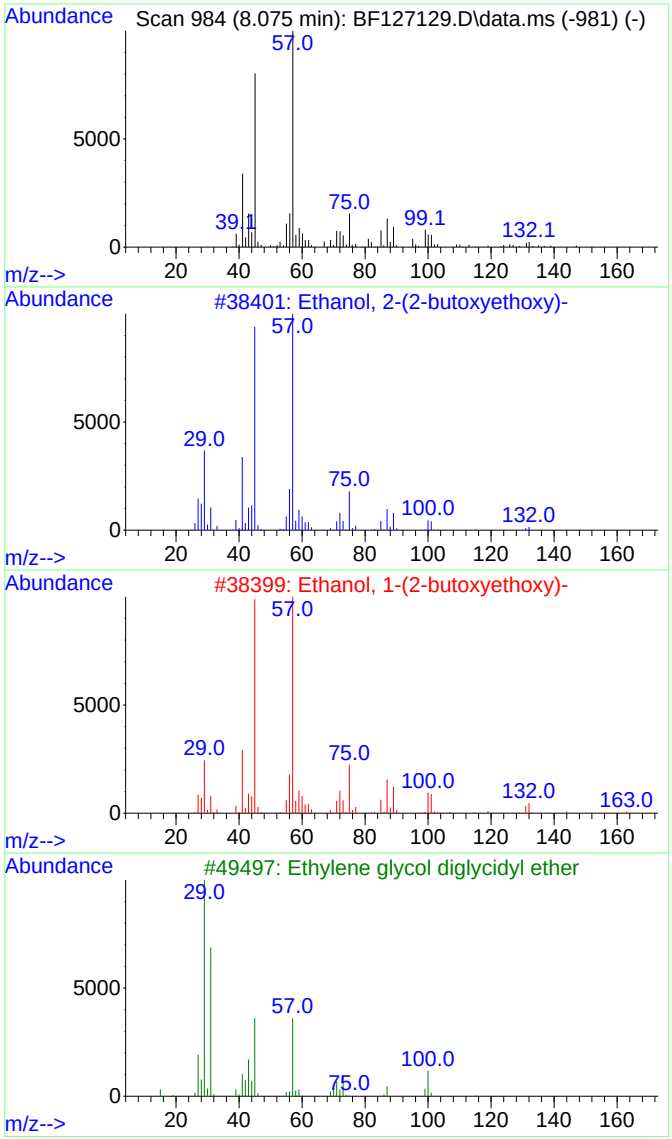
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

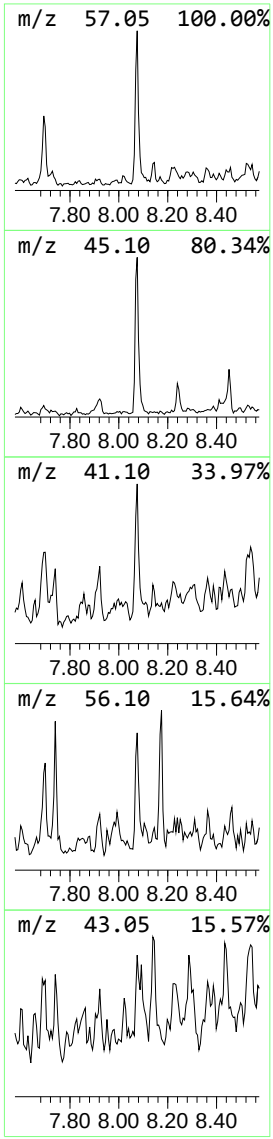
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	4.43 ng	158250	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	59
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	58





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Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

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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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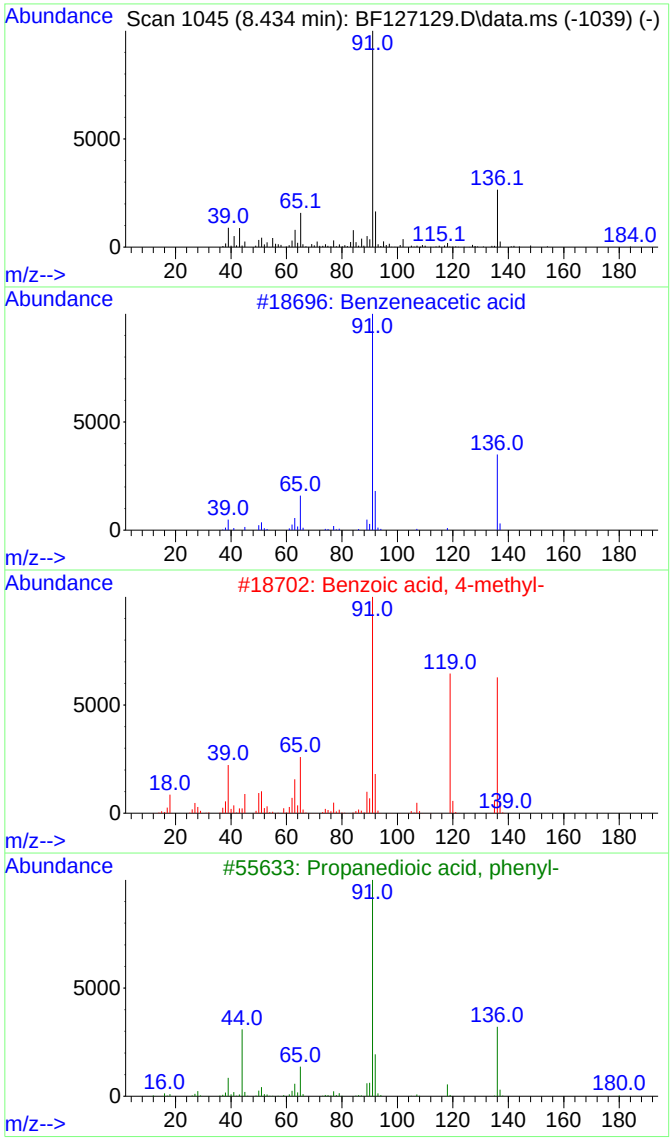
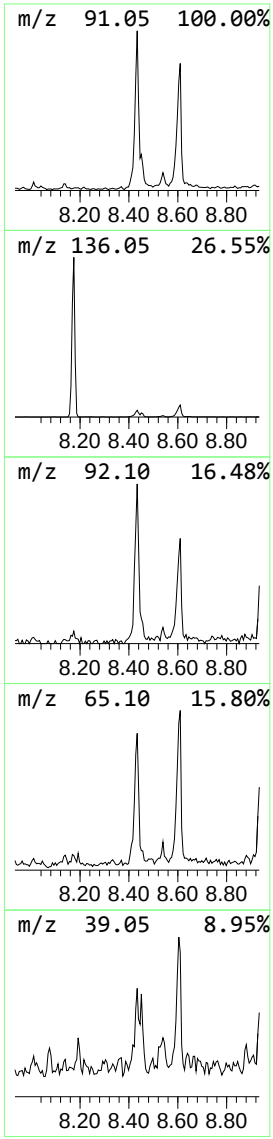
Peak Number 10 Benzeneacetic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	6.10 ng	218174	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	52
3	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	50
4	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	43
5	.alpha.-Nitrodibenzyl sulfone	291	C14H13NO4S	021272-80-0	43





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

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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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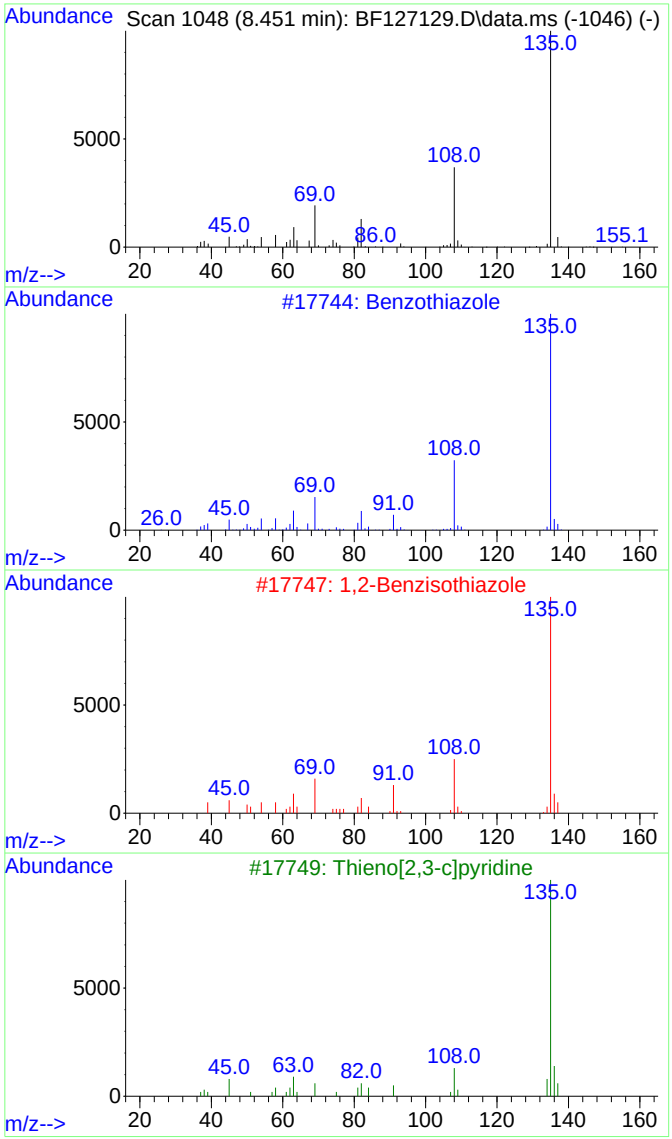
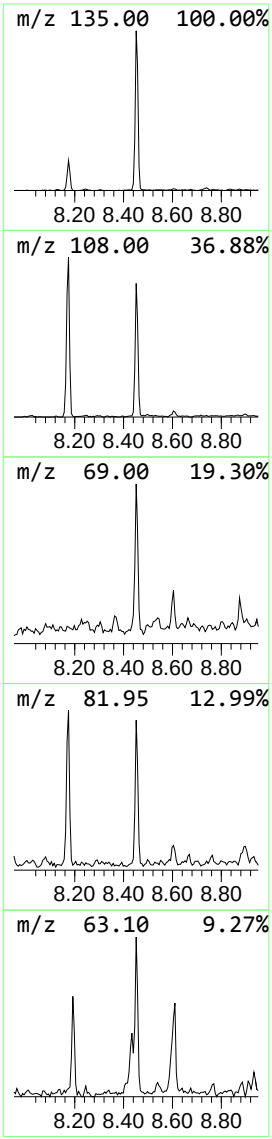
Peak Number 11 Benzothiazole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	8.27 ng	295568	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	91
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	86
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	64
4	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	59
5	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	56





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Sample : N1688-12
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ALS Vial : 17 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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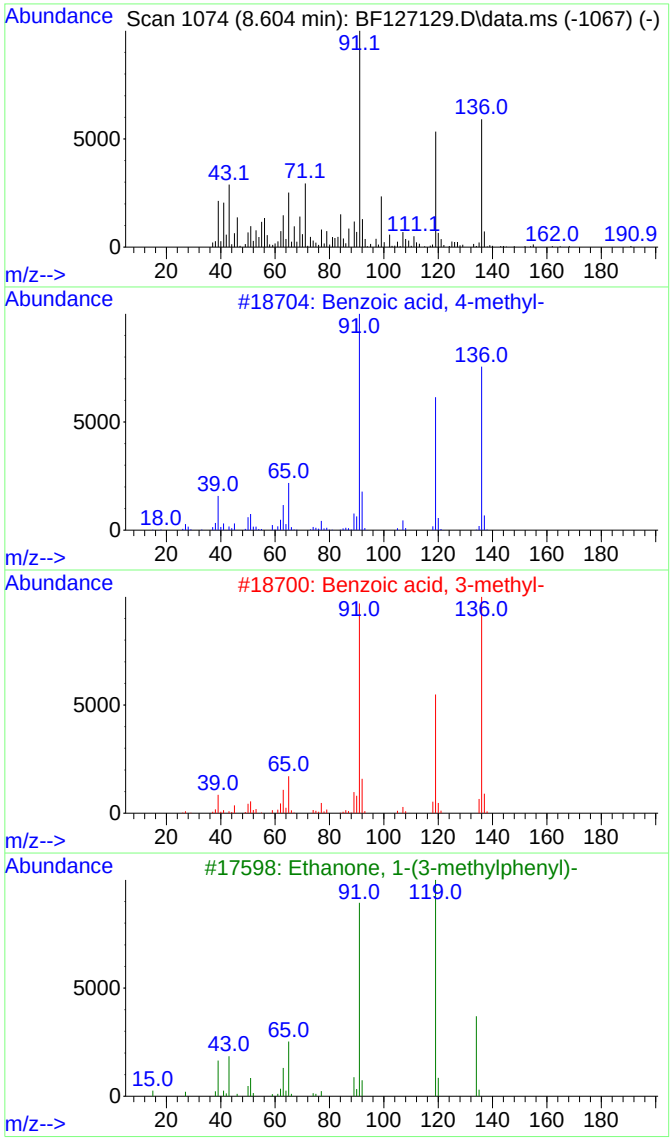
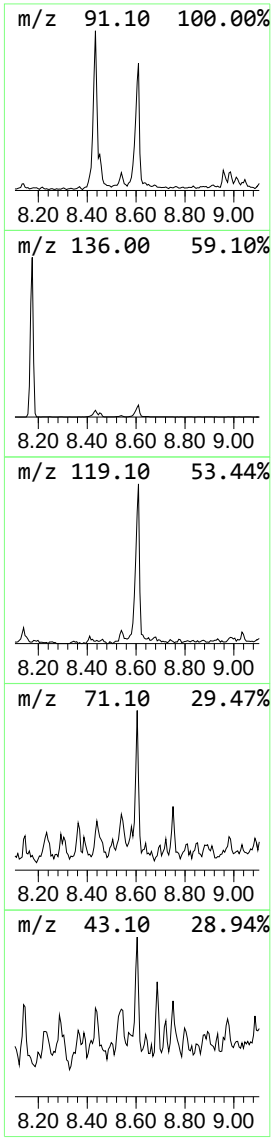
Peak Number 12 Benzoic acid, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.604	10.25 ng	366725	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	93
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	52
3	Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	43
4	Benzeneacetic acid	136	C8H8O2	000103-82-2	41
5	Benzoyl chloride, 4-methyl-	154	C8H7ClO	000874-60-2	38





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Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

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BNA_F
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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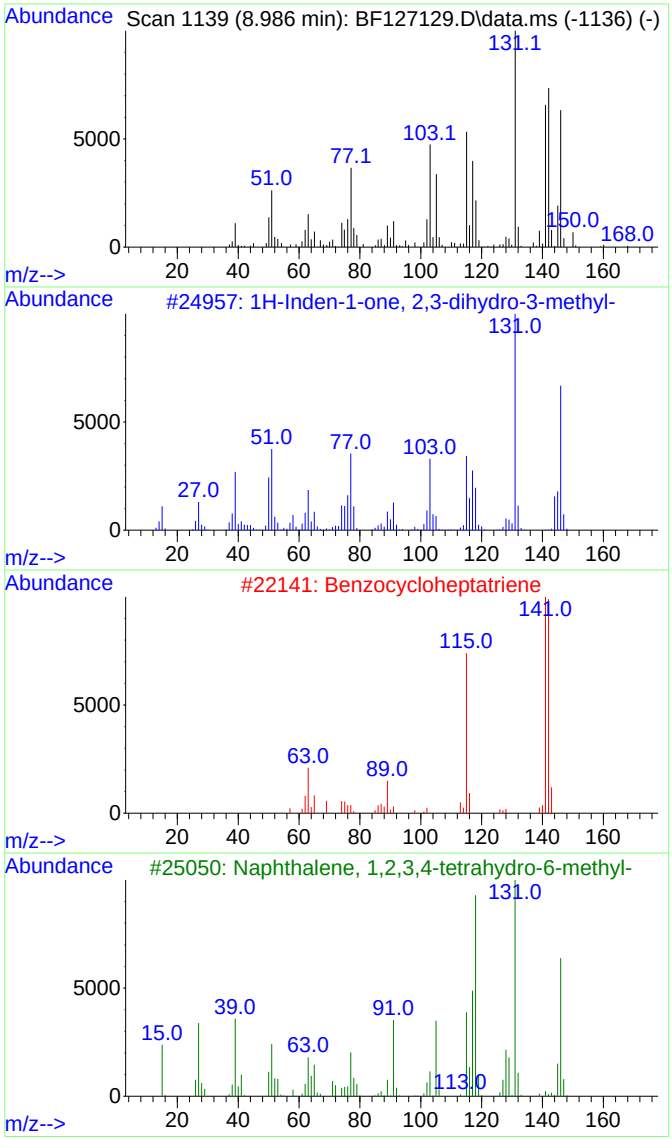
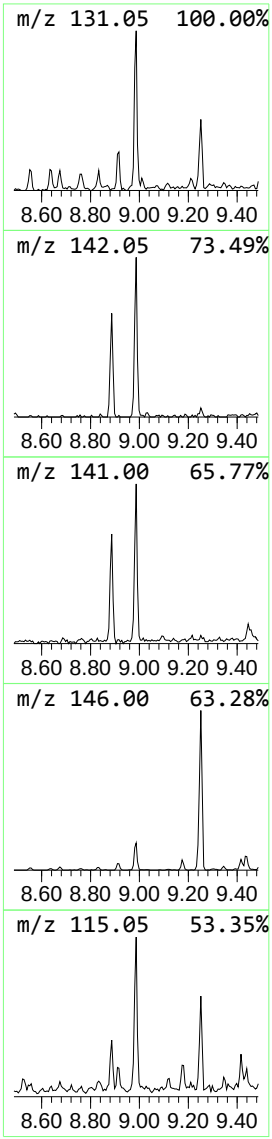
Peak Number 13 1H-Inden-1-one, 2,3-dihydro... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.986	5.85 ng	209257	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	64
2	Benzocycloheptatriene	142	C11H10	000264-09-5	56
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	45
4	1-Methylindan-2-one	146	C10H10O	035587-60-1	43
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	42





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Operator : CG\JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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BNA_F
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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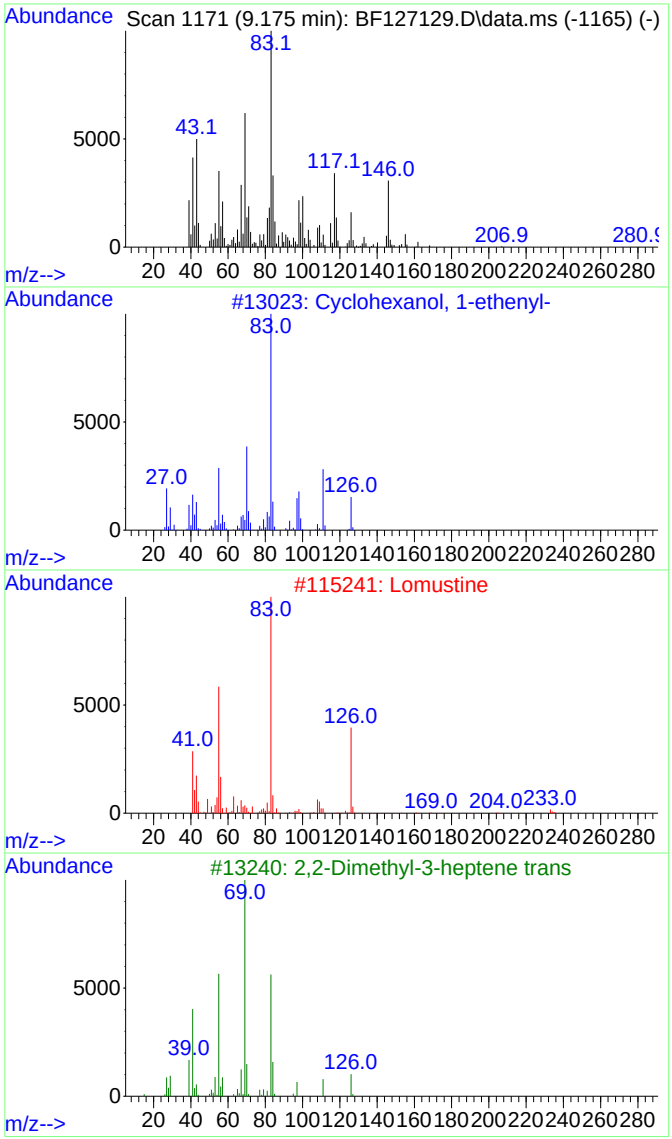
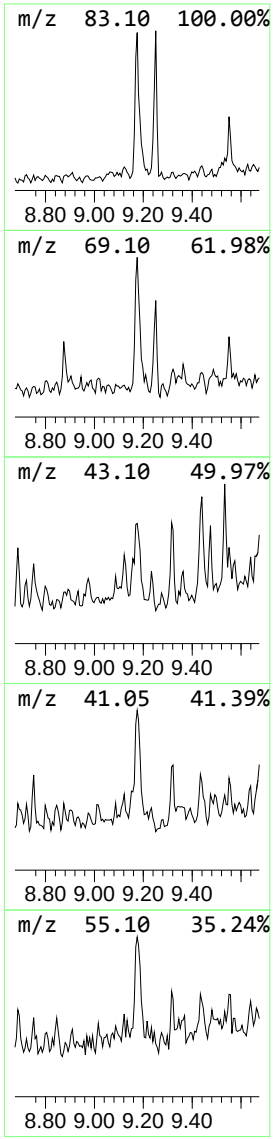
Peak Number 14 unknown9.175 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.175	7.88 ng	288018	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 1-ethenyl-	126	C8H14O	001940-19-8	43
2	Lomustine	233	C9H16ClN3O2	013010-47-4	38
3	2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	38
4	5-Oxa-6-azaspiro[3.4]oct-6-ene	111	C6H9NO	1000362-18-0	38
5	3-Methyl-2-butenoic acid, 2-pent...	170	C10H18O2	150462-84-3	35





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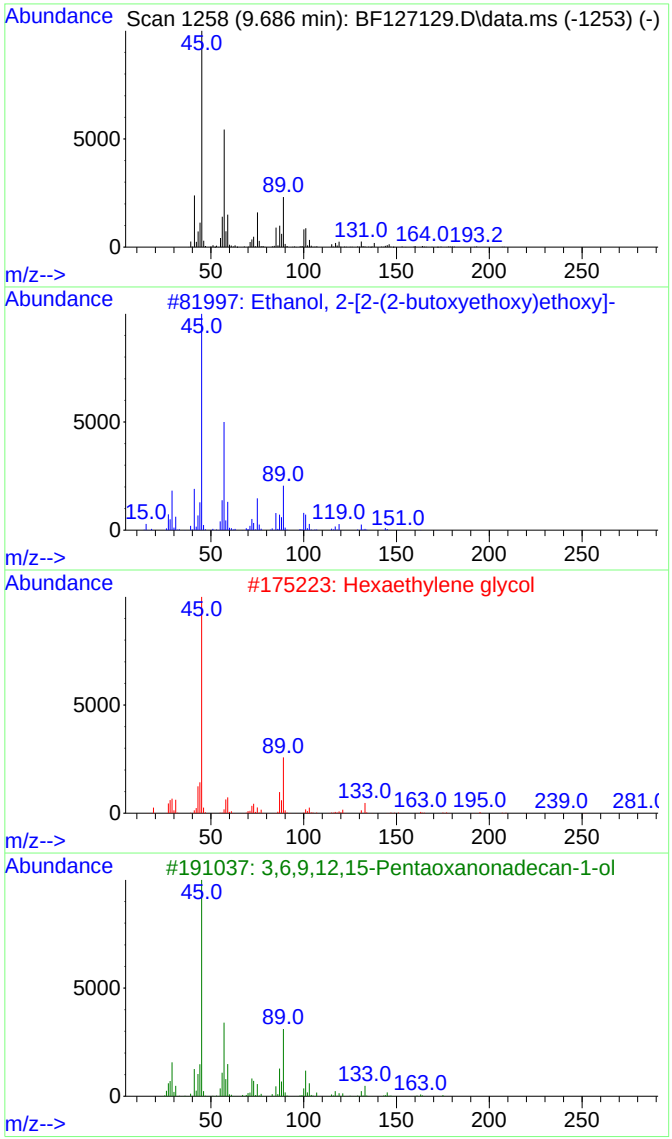
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

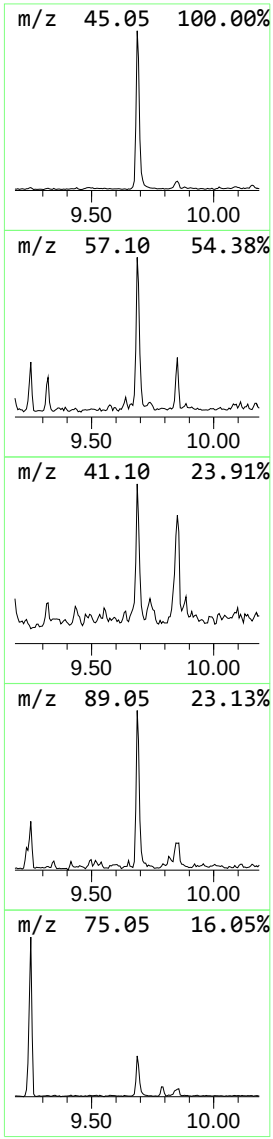
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.686	11.19 ng	409089	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	91
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	72
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	72
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	64
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	64





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Sample : N1688-12
Misc :
ALS Vial : 17 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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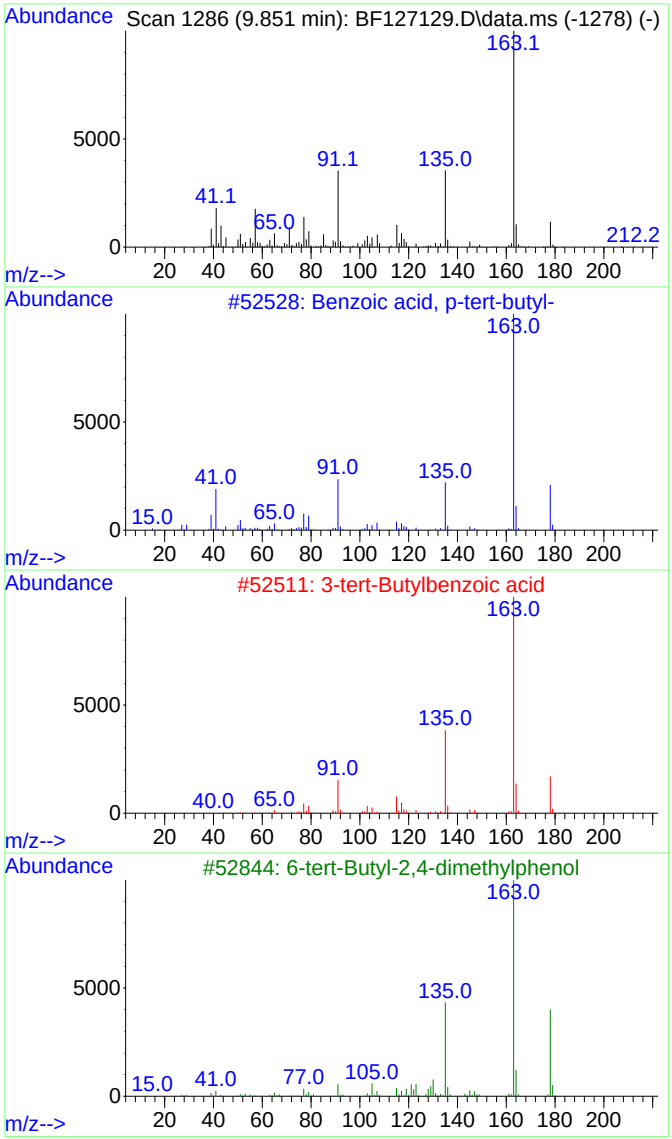
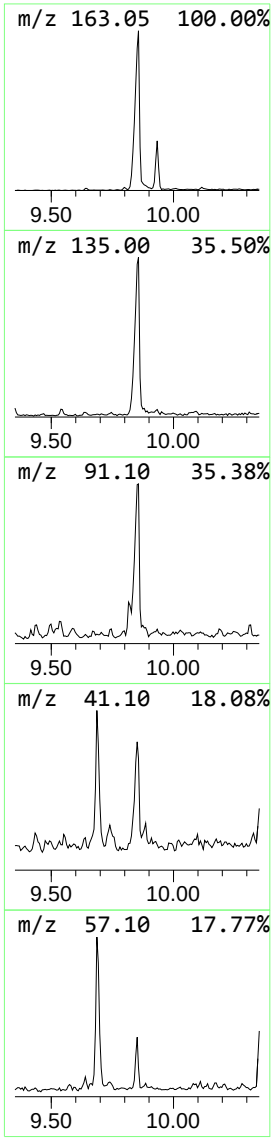
Peak Number 16 Benzoic acid, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	18.82 ng	688057	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	78
3	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
4	3-pyridinecarbonitrile, 2-amino-...	163	C8H9N3O	1010404-44-3	64
5	5-Fluoro-8-quinolinol	163	C9H6FNO	000387-97-3	59





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Sample : N1688-12
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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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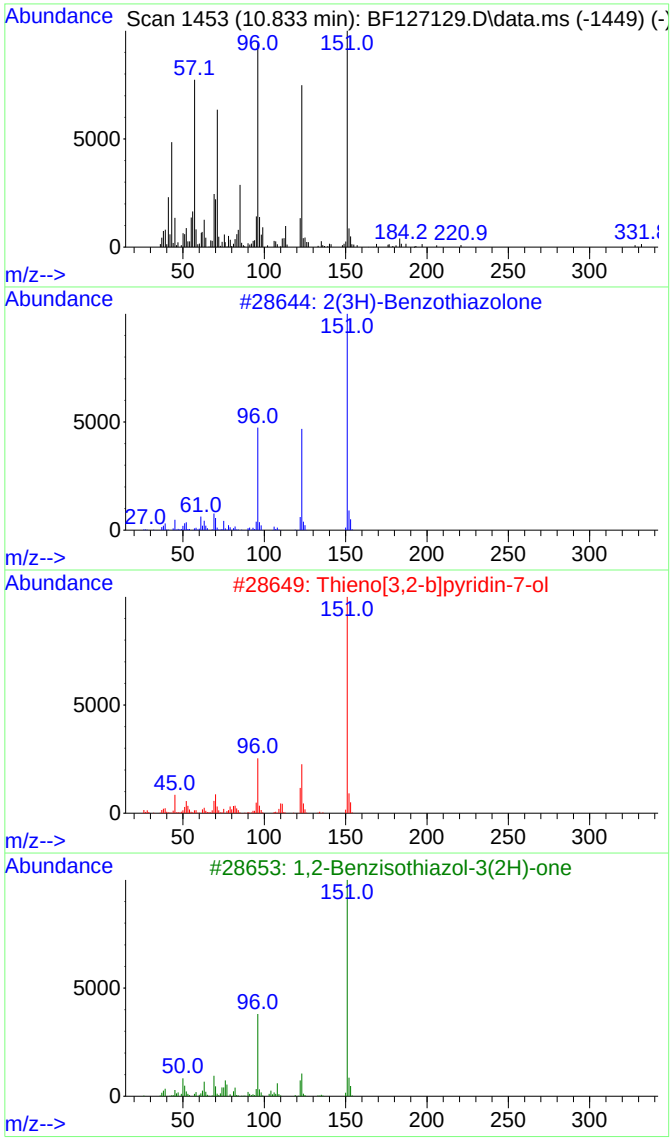
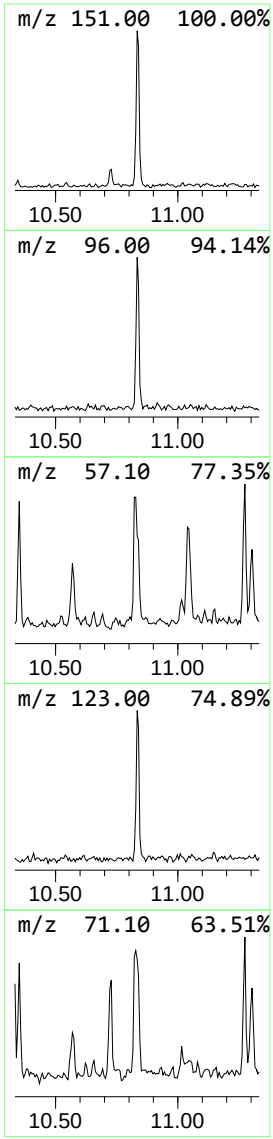
Peak Number 17 2(3H)-Benzothiazolone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.833	7.83 ng	257574	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	68
2	Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	49
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	43
4	Benzene, fluoro-	96	C6H5F	000462-06-6	11
5	1,2,4-Triazolo[4,3-a]pyridine-3(...	151	C6H5N3S	006952-68-7	11





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ALS Vial : 17 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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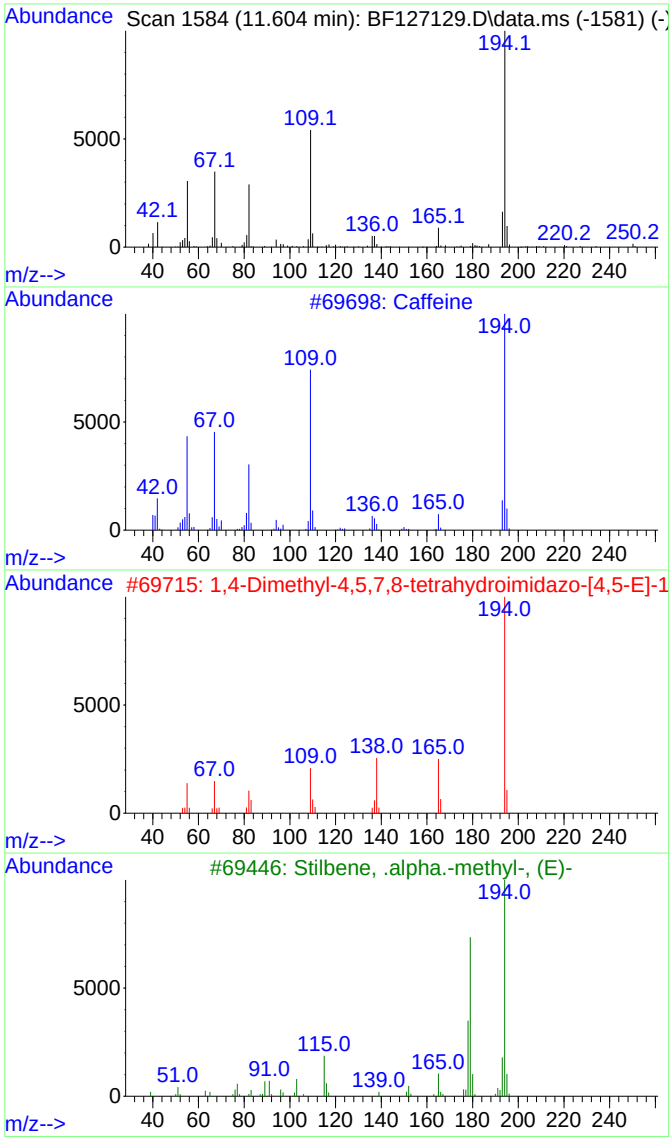
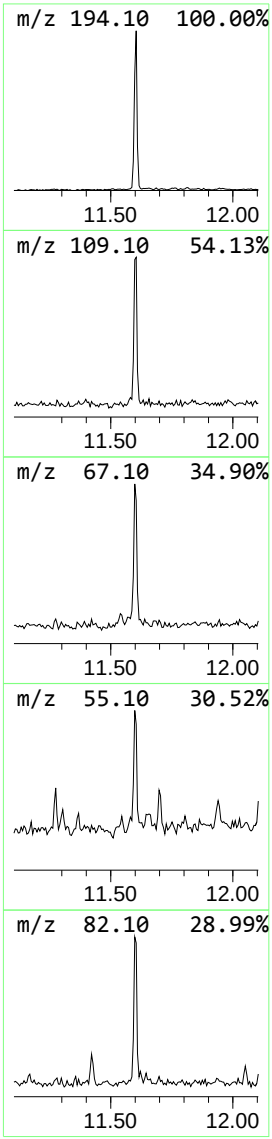
Peak Number 18 Caffeine Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	5.06 ng	166552	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	96
2	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	53
3	Stilbene, .alpha.-methyl-, (E)-	194	C15H14	000833-81-8	43
4	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	40
5	Benzaldehyde, 4,6-dimethoxy-2,3-...	194	C11H14O3	034883-13-1	38





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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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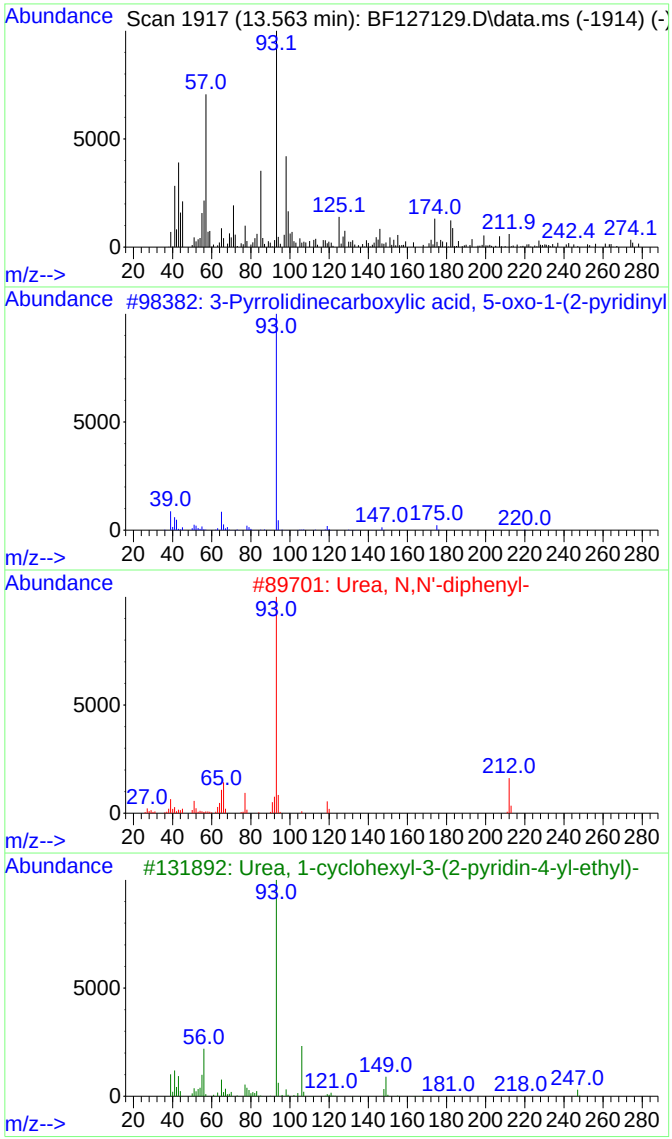
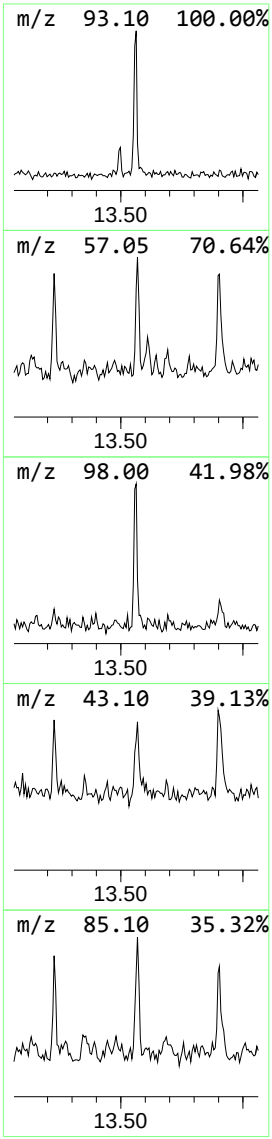
Peak Number 19 unknown13.563 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.563	6.15 ng	116527	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyrrolidinecarboxylic acid, 5-...	220	C11H12N2O3	1000337-74-3	38
2	Urea, N,N'-diphenyl-	212	C13H12N2O	000102-07-8	30
3	Urea, 1-cyclohexyl-3-(2-pyridin-...	247	C14H21N3O	1000310-78-3	27
4	isobutyranilide	163	C10H13NO	004406-41-1	27
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	22





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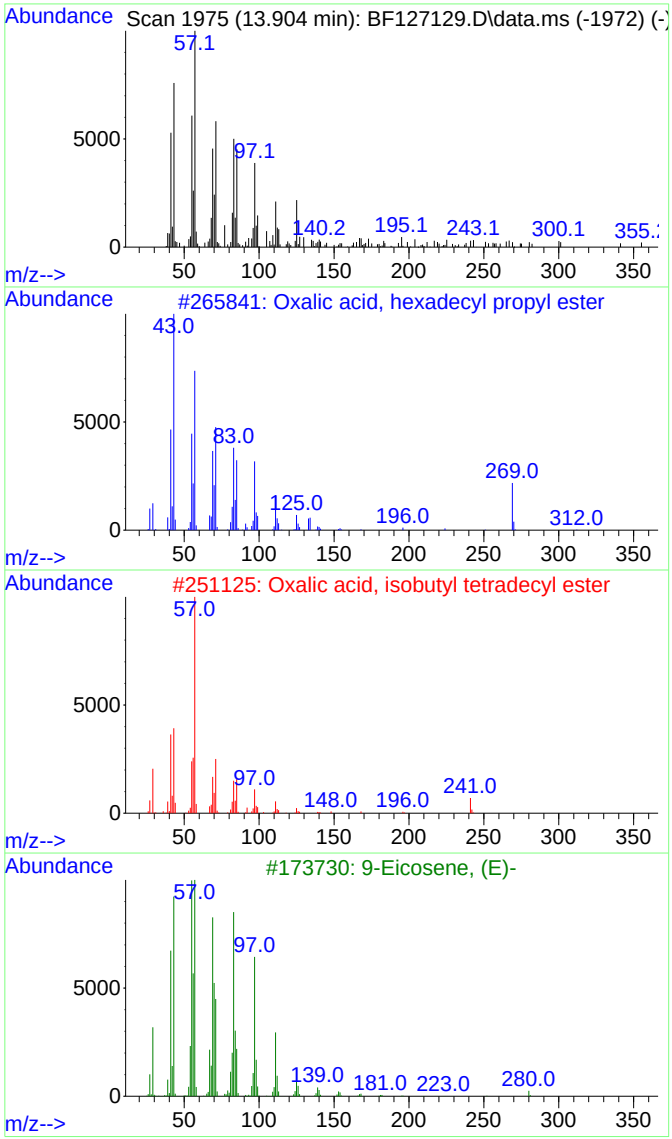
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

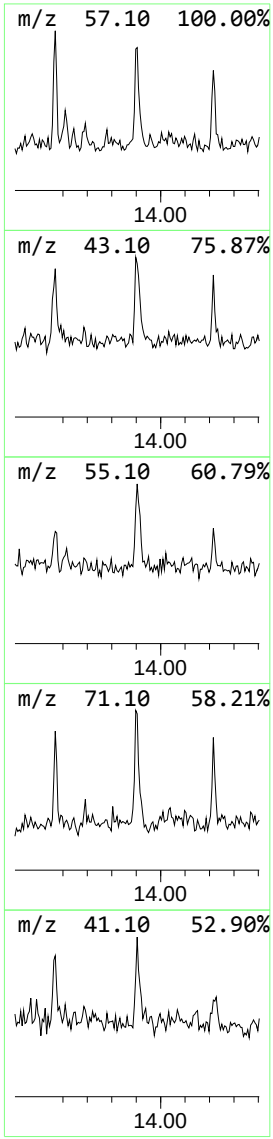
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Oxalic acid, hexadecyl prop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.91 ng	111976	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	87
2	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	87
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	83
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030122\
Data File : BF127129.D
Acq On : 01 Mar 2022 21:25
Operator : CG\JU
Sample : N1688-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Hexanoic acid	5.187	4.5	ng	118738	1	6.887	525171	20.0
Benzene, 1-ethy...	6.445	5.1	ng	135001	1	6.887	525171	20.0
Mesitylene	6.710	21.1	ng	554801	1	6.887	525171	20.0
Benzene, 1,2,3-...	6.945	13.4	ng	351540	1	6.887	525171	20.0
Indane	7.069	8.5	ng	224128	1	6.887	525171	20.0
Ethanol, 2-(2-b...	8.075	4.4	ng	158250	2	8.175	715226	20.0
Benzeneacetic acid	8.434	6.1	ng	218174	2	8.175	715226	20.0
Benzothiazole	8.451	8.3	ng	295568	2	8.175	715226	20.0
Benzoic acid, 4...	8.604	10.3	ng	366725	2	8.175	715226	20.0
1H-Inden-1-one,...	8.986	5.8	ng	209257	2	8.175	715226	20.0
unknown9.175	9.175	7.9	ng	288018	3	9.933	731054	20.0
Ethanol, 2-[2-(...	9.686	11.2	ng	409089	3	9.933	731054	20.0
Benzoic acid, p...	9.851	18.8	ng	688057	3	9.933	731054	20.0
2(3H)-Benzothia...	10.833	7.8	ng	257574	4	11.422	658207	20.0
Caffeine	11.604	5.1	ng	166552	4	11.422	658207	20.0
unknown13.563	13.563	6.2	ng	116527	5	14.068	378791	20.0
Oxalic acid, he...	13.904	5.9	ng	111976	5	14.068	378791	20.0