LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW1

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054887.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.846	87	95	101	rVB	17652	27576	1.11%	0.223%
2	5.203	318	326	333	rBV3	18991	39709	1.60%	0.321%
3	5.691	402	409	422	rVB	213834	363401	14.63%	2.939%
4	7.300	676	683	694	rBV	132961	241865	9.73%	1.956%
5	8.147	820	827	833	rBV	111024	192262	7.74%	1.555%
6	9.322	1019	1027	1042	rVB	327770	609440	24.53%	4.929%
7	10.726	1257	1266	1280	rBV3	12582	38288	1.54%	0.310%
8	10.973	1300	1308	1314	rBV	151593	287983	11.59%	2.329%
9	12.794	1612	1618	1623	rBV	23982	40500	1.63%	0.328%
10	13.047	1656	1661	1666	rBV2	24651	37959	1.53%	0.307%
11	13.211	1681	1689	1699	rBV6	12353	35818	1.44%	0.290%
12	13.323	1704	1708	1713	rVV2	15437	25800	1.04%	0.209%
13	13.405	1713	1722	1729	rVB	986440	1575560	63.41%	12.742%
14	13.975	1815	1819	1823	rBV4	18896	26438	1.06%	0.214%
15	14.269	1865	1869	1875	rVB6	19284	36121	1.45%	0.292%
16	14.416	1889	1894	1904	rVB	83193	125656	5.06%	1.016%
17	14.786	1951	1957	1970	rVB	263944	466767	18.79%	3.775%
18	14.892	1970	1975	1979	rBV3	17053	28897	1.16%	0.234%
19	14.939	1979	1983	1991	rVB10	20469	35021	1.41%	0.283%
20	15.262	2034	2038	2042	rVV4	25016	35656	1.44%	0.288%
21	15.315	2044	2047	2051	rVV4	17287	29083	1.17%	0.235%
22	15.373	2052	2057	2066	rVB	166435	254558	10.25%	2.059%
23	15.579	2087	2092	2103	rVB	110707	183212	7.37%	1.482%
24	15.796	2125	2129	2135	rBV4	44729	72368	2.91%	0.585%
25	15.890	2141	2145	2149	rBV5	22841	32682	1.32%	0.264%
26	16.014	2162	2166	2169	rBV3	19498	28195	1.13%	0.228%
27	16.055	2169	2173	2176	rVV	54913	65303	2.63%	0.528%
28	16.102	2178	2181	2185	rVV2	32966	50010	2.01%	0.404%
29	16.149	2185	2189	2198	rVB6	38662	91012	3.66%	0.736%
30	16.237	2199	2204	2205	rBV	61322	83824	3.37%	0.678%
31	16.272	2205	2210	2217	rVB	779636	1213446	48.84%	9.814%
32	16.419	2231	2235	2243	rVB3	39309	69812	2.81%	0.565%
33	16.525	2249	2253	2257	rVB7	17945	26526	1.07%	0.215%
34	16.601	2261	2266	2272	rBV5	36293	58659	2.36%	0.474%
35	16.766	2289	2294	2297	rBV2	51889	81735	3.29%	0.661%
36	16.795	2297	2299	2305	rVB2	46655	61825	2.49%	0.500%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.889	2311	2315	2324	rVB3	69227	109766	4.42%	0.888%
38	16.966	2324	2328	2333	rBV	41387	53826	2.17%	0.435%
39	17.089	2345	2349	2353	rVB4	34966	47589	1.92%	0.385%
40	17.530	2419	2424	2432	rVB	339030	528239	21.26%	4.272%
41	17.724	2452	2457	2468	rBV5	113033	225443	9.07%	1.823%
42	18.082	2514	2518	2522	rBV5	29694	47407	1.91%	0.383%
43	18.288	2549	2553	2562	rVB3	52446	109702	4.42%	0.887%
44	18.399	2569	2572	2581	rBV10	20874	39541	1.59%	0.320%
45	18.599	2603	2606	2615	rVB3	25028	38716	1.56%	0.313%
46	19.915	2827	2830	2834	rBV	40618	52117	2.10%	0.421%
47	20.132	2861	2867	2874	rVB	1829648	2484643	100.00%	20.095%
48	20.409	2912	2914	2917	rVB	30851	28681	1.15%	0.232%
49	20.908	2996	2999	3003	rVB	70564	76619	3.08%	0.620%
50	21.431	3084	3088	3094	rVB	86967	119270	4.80%	0.965%
51	21.830	3150	3156	3163	rVB2	348432	590391	23.76%	4.775%
52	21.924	3168	3172	3177	rVB5	52587	86208	3.47%	0.697%
53	21.989	3179	3183	3190	rVB	61462	105730	4.26%	0.855%
54	22.624	3287	3291	3297	rBV	44344	70194	2.83%	0.568%
55	23.352	3411	3415	3421	rVB2	38147	73231	2.95%	0.592%
56	23.552	3444	3449	3456	rVB2	53364	102295	4.12%	0.827%
57	25.209	3722	3731	3746	rVB2	229744	702124	28.26%	5.678%

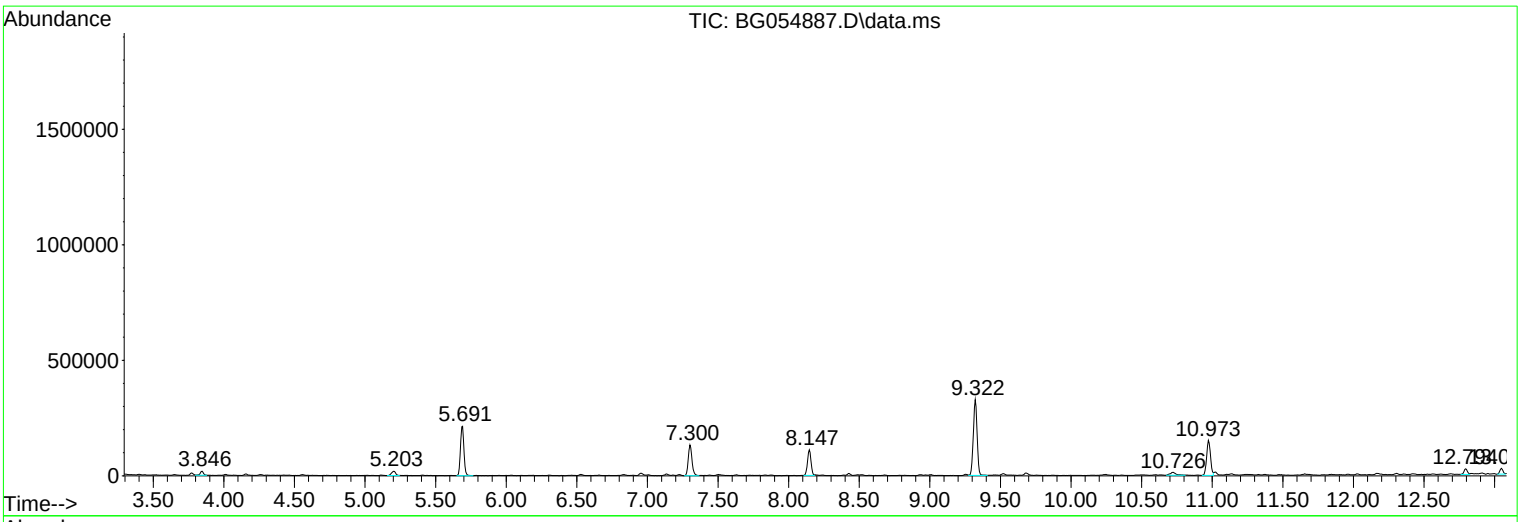
Sum of corrected areas: 12364699

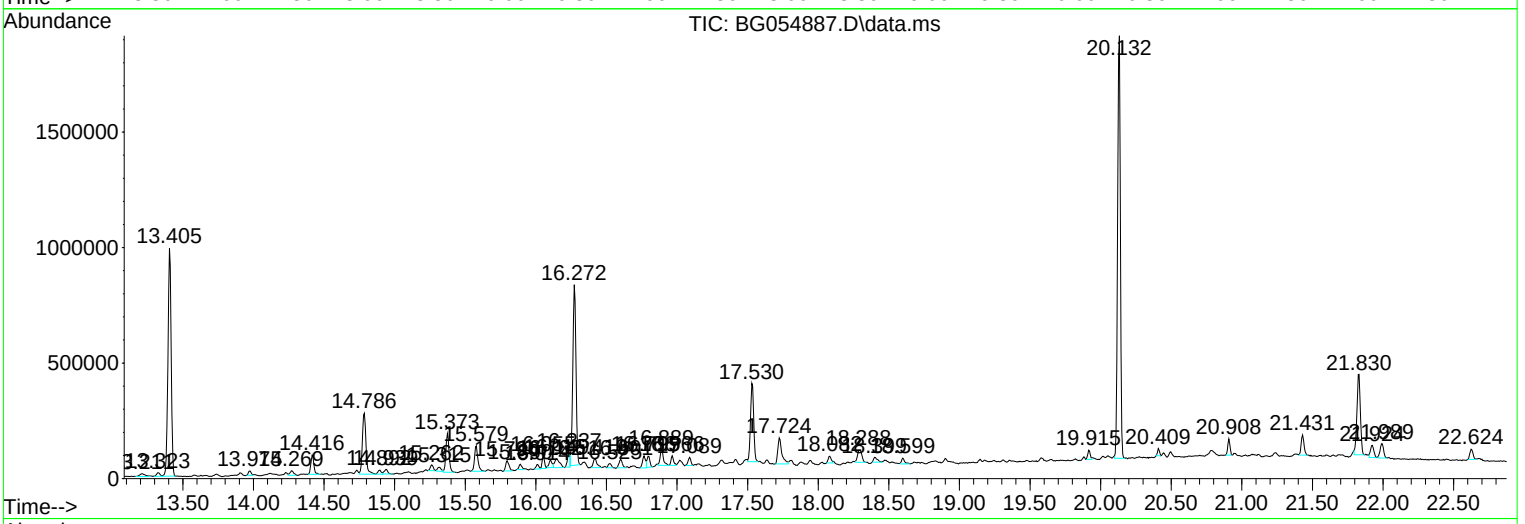
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

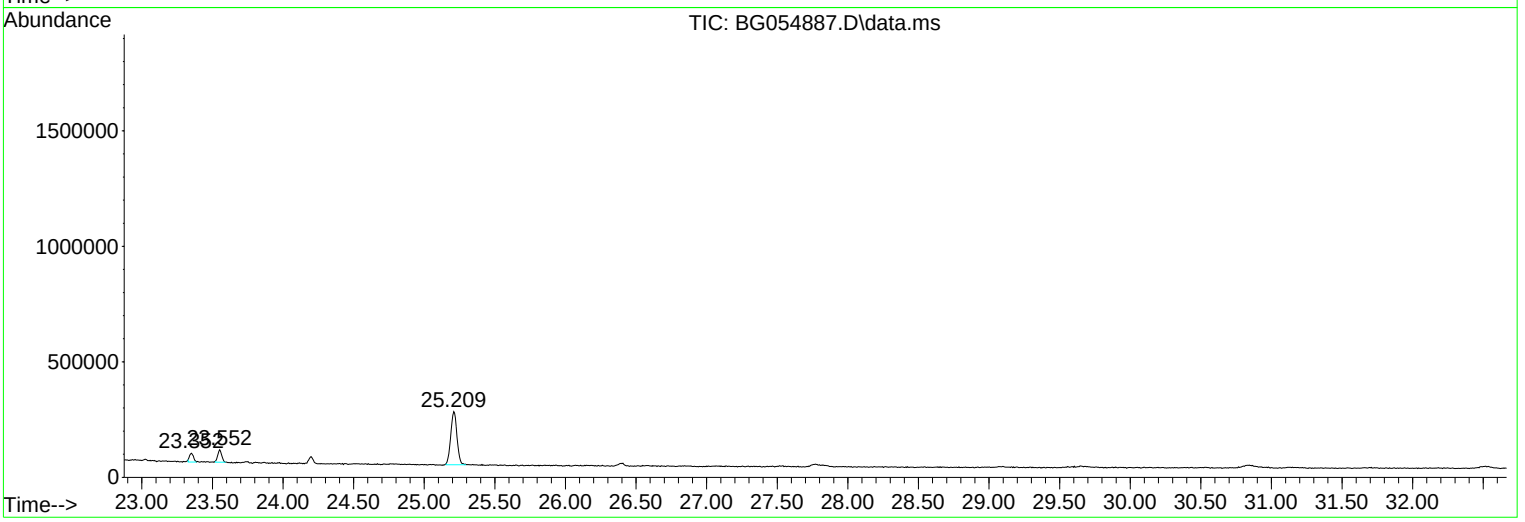
Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

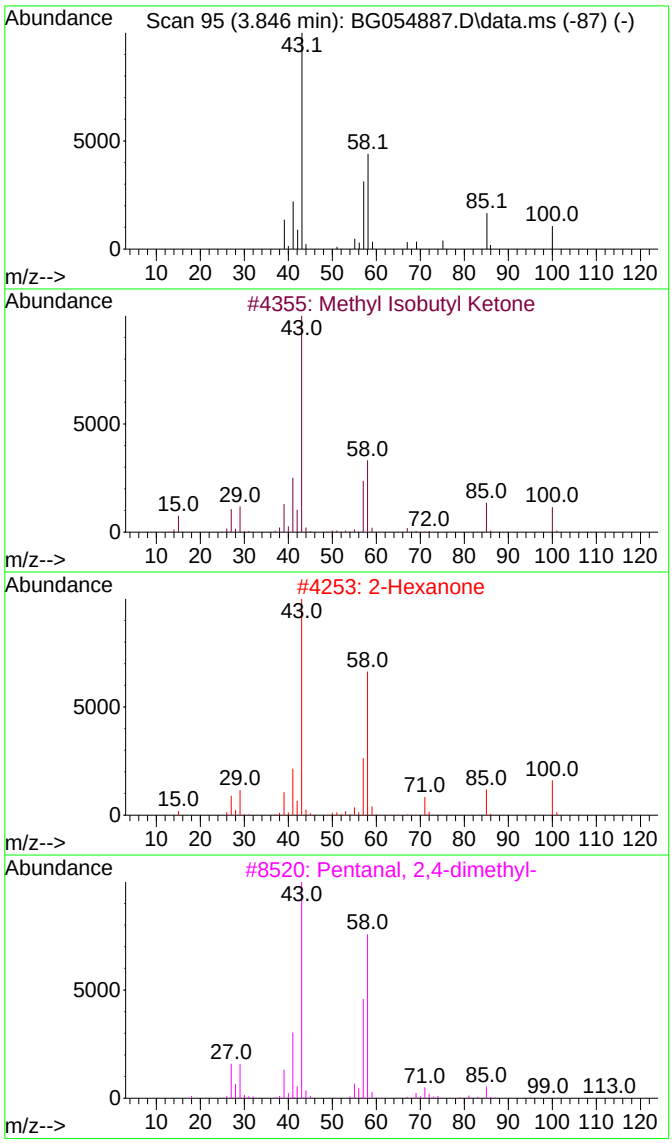
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

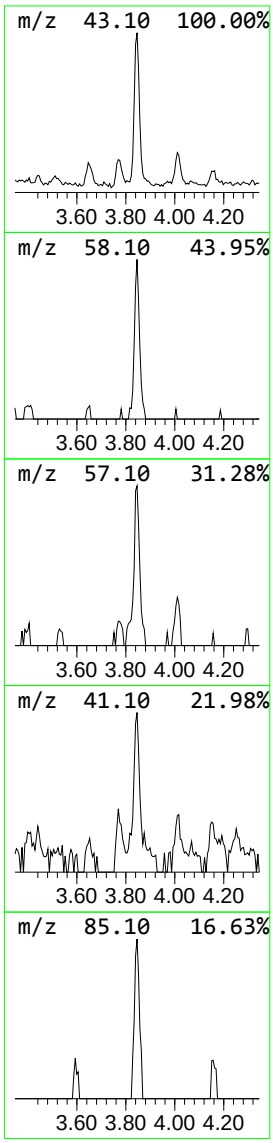
****

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.846	2.87 ng	27576	1,4-Dichlorobenzene-d4	8.147

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	80
2	2-Hexanone	100	C6H12O	000591-78-6	64
3	Pentanal, 2,4-dimethyl-	114	C7H14O	027944-79-2	33
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	25
5	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

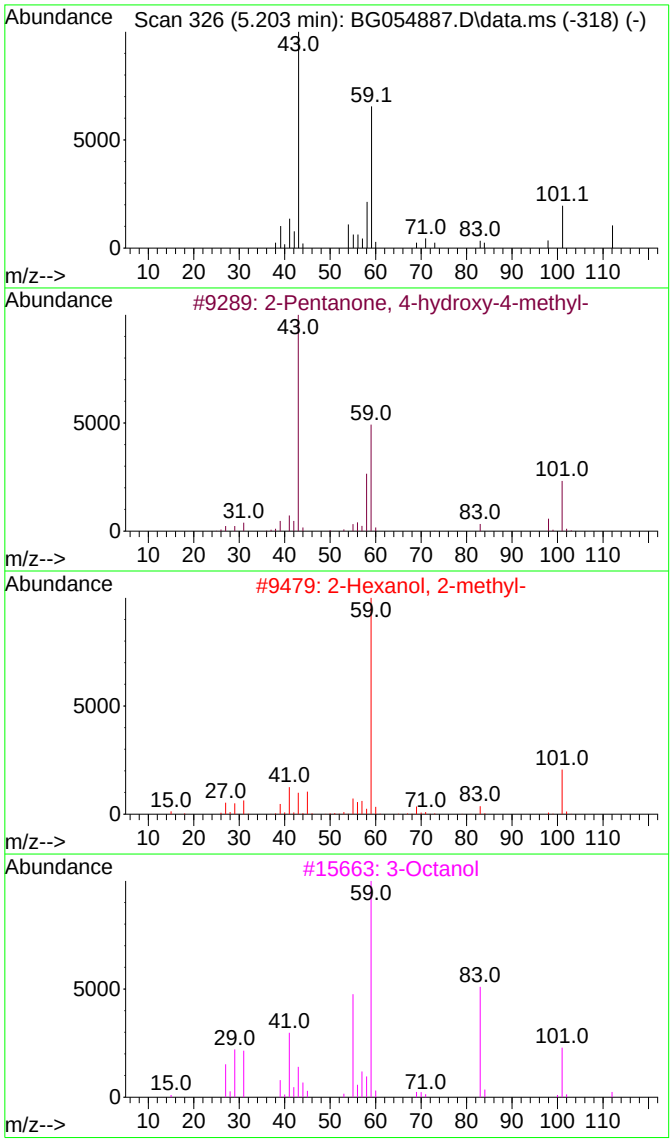
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

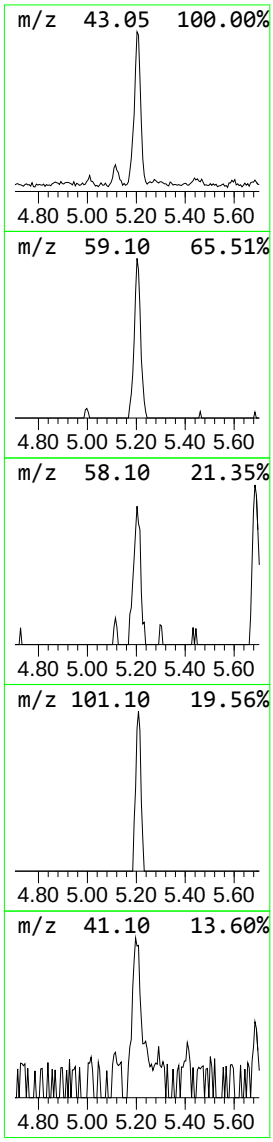
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.203	4.13 ng	39709	1,4-Dichlorobenzene-d4	8.147

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	35
3	3-Octanol	130	C8H18O	000589-98-0	23
4	3-Octanol, acetate	172	C10H20O2	004864-61-3	17
5	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

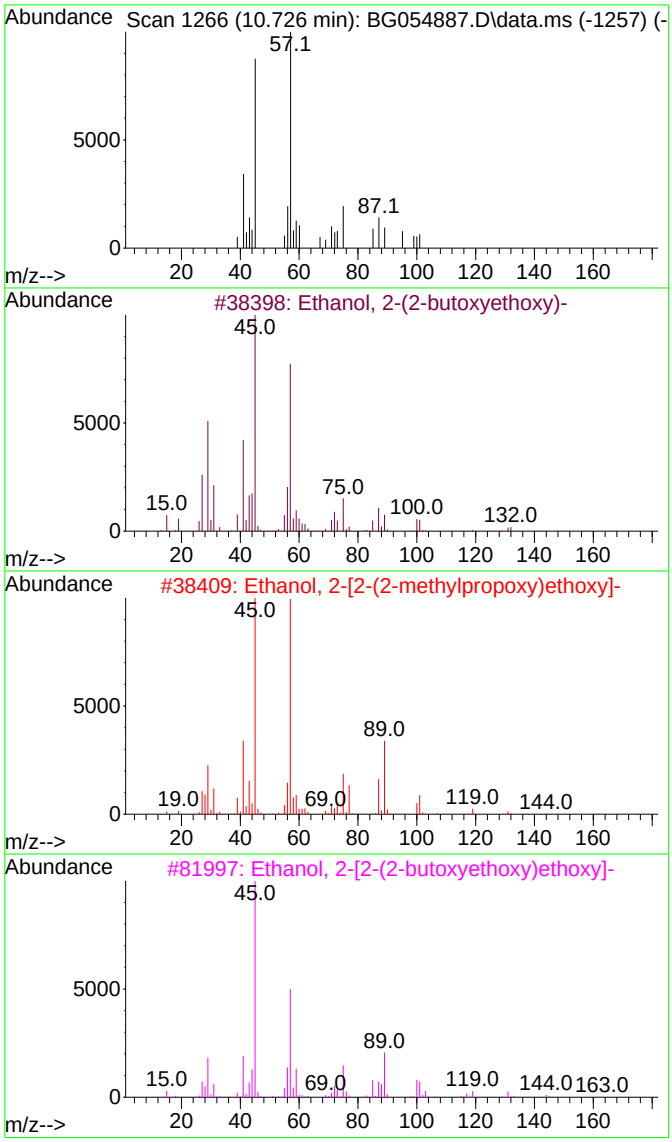
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

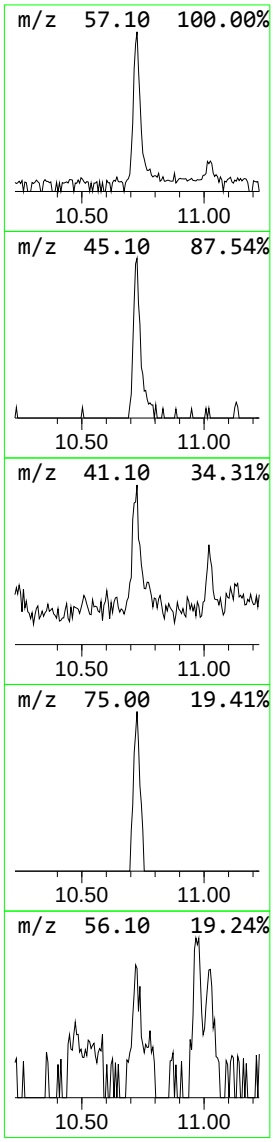
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.726	2.66 ng	38288	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	53
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

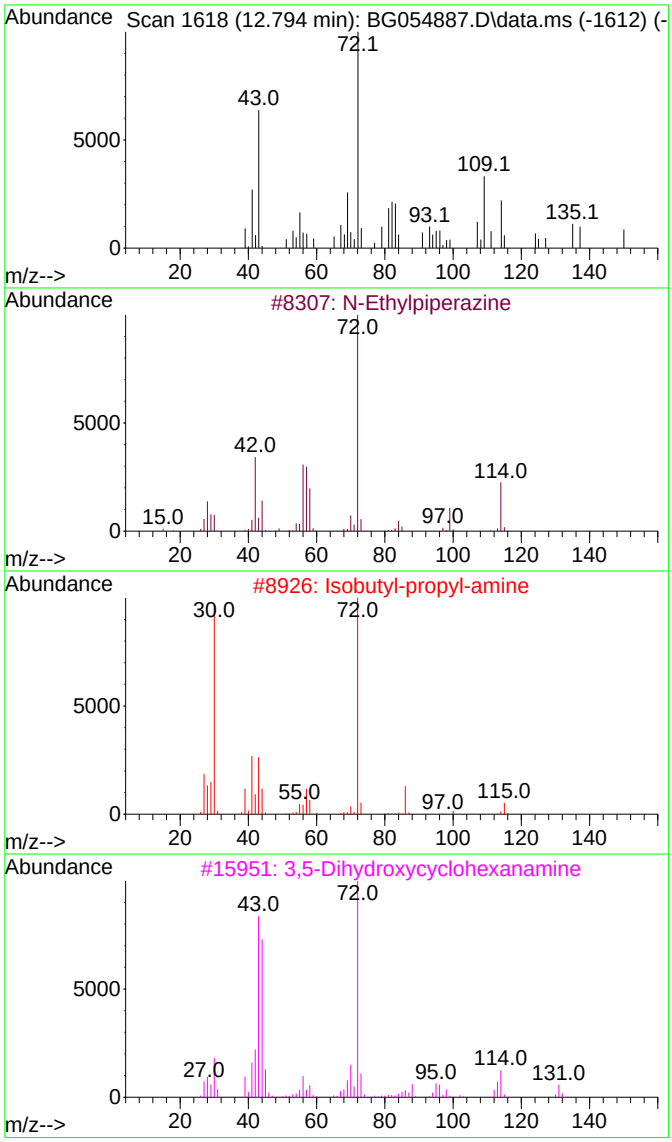
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

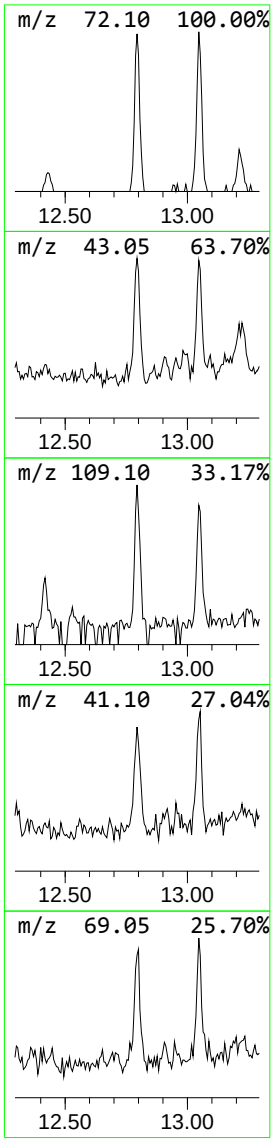
****

Peak Number 4 unknown12.794 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.794	2.81 ng	40500	Naphthalene-d8	10.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Ethylpiperazine	114	C6H14N2	005308-25-8	38
2	Isobutyl-propyl-amine	115	C7H17N	039190-66-4	27
3	3,5-Dihydroxycyclohexanamine	131	C6H13NO2	1000192-83-1	25
4	2-Propanol, 1-(isopropylamino)-3...	239	C13H21NOS	019343-26-1	25
5	2,4-Pentanedione, 3-methyl-	114	C6H10O2	000815-57-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

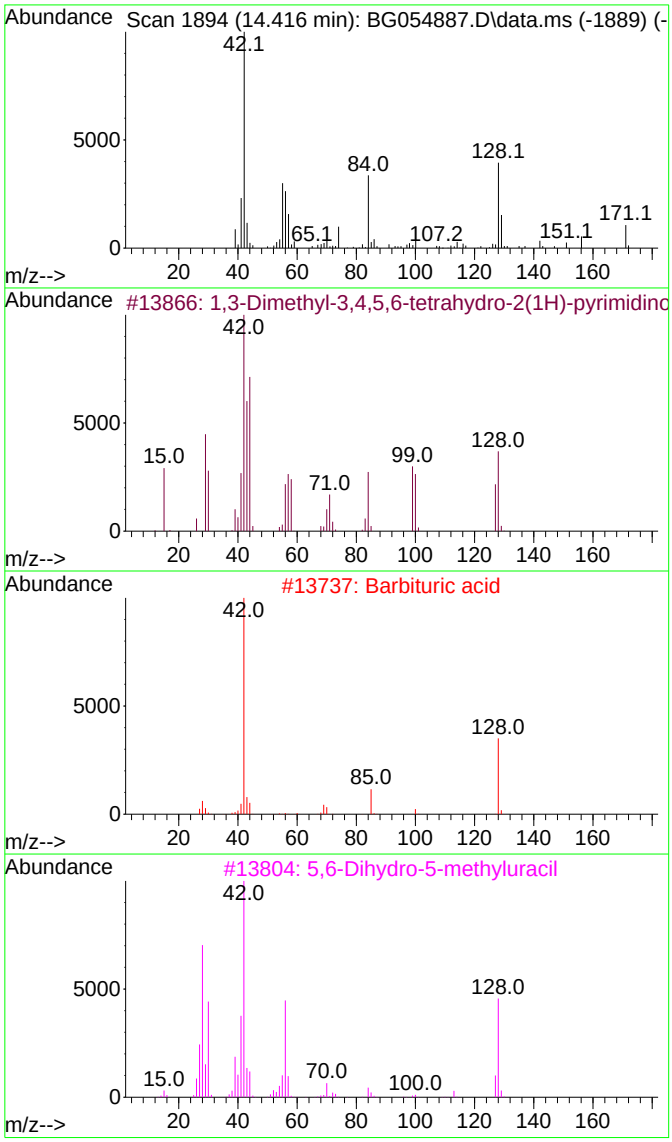
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

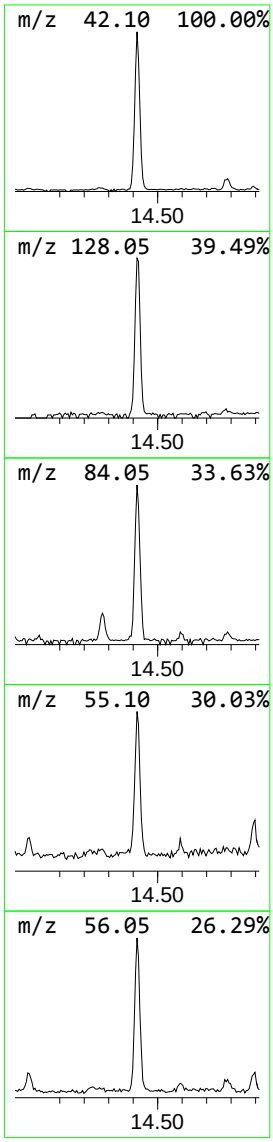
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dimethyl-3,4,5,6-tetrah... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	5.38 ng	125656	Acenaphthene-d10	14.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-3,4,5,6-tetrahydro-...	128	C6H12N2O	007226-23-5	50
2	Barbituric acid	128	C4H4N2O3	000067-52-7	40
3	5,6-Dihydro-5-methyluracil	128	C5H8N2O2	000696-04-8	33
4	Acetaldehyde, ethylidenehydrazone	84	C4H8N2	000592-56-3	32
5	1,2,4,5-Tetrazine, 1,4-dihydro-3...	112	C4H8N4	037454-64-1	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

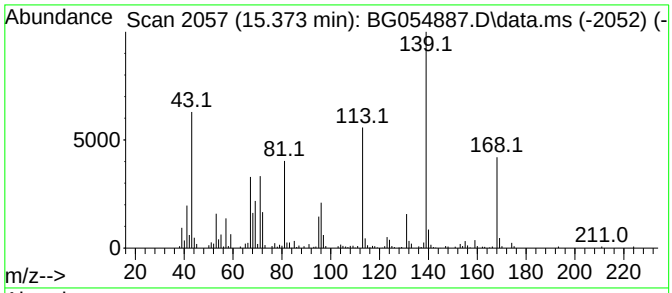
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

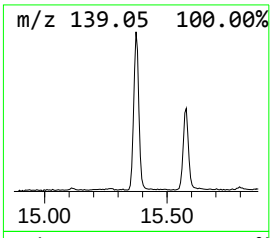
****

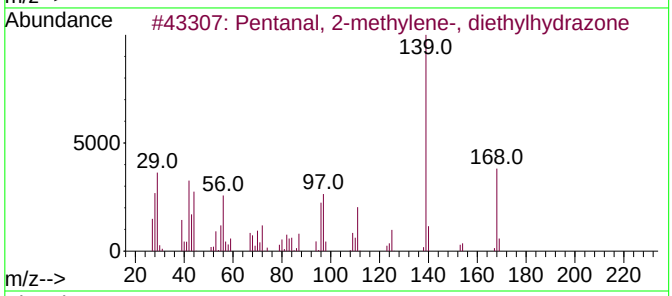
Peak Number 6 unknown15.373 Concentration Rank 1

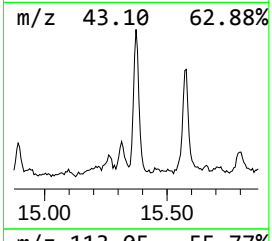
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.373	10.91 ng	254558	Acenaphthene-d10	14.786

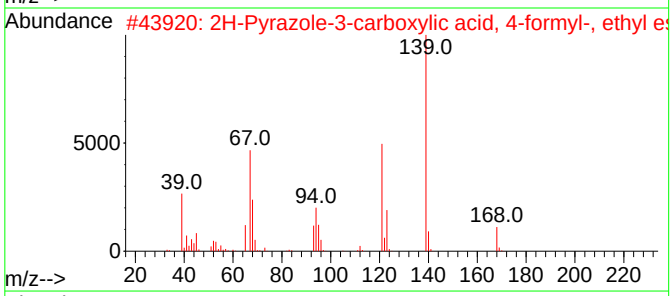
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal, 2-methylene-, diethylh...	168	C10H20N2	025186-14-5	46
2	2H-Pyrazole-3-carboxylic acid, 4...	168	C7H8N2O3	1000302-22-0	43
3	4-Fluoro-N1-propyl-1,2-benzenedi...	168	C9H13FN2	300798-95-2	35
4	2-Carboxamidopyrazine 4-N-oxide	139	C5H5N3O2	000768-36-5	27
5	Pyrazinecarboxamide, 3,4-dihydro...	139	C5H5N3O2	055321-99-8	27

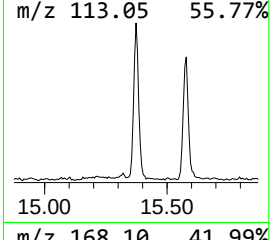


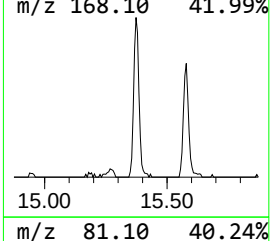


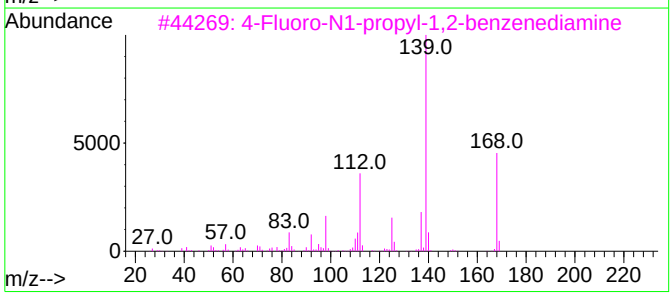


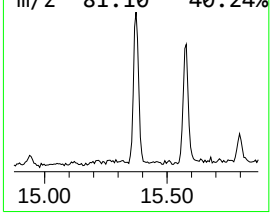












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

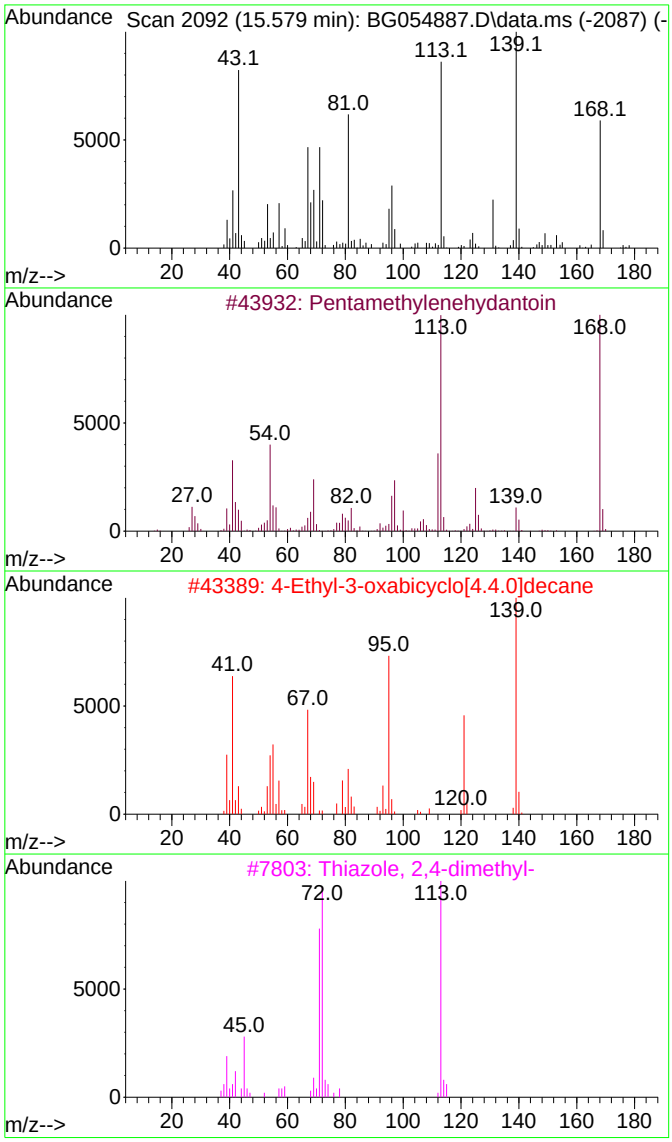
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

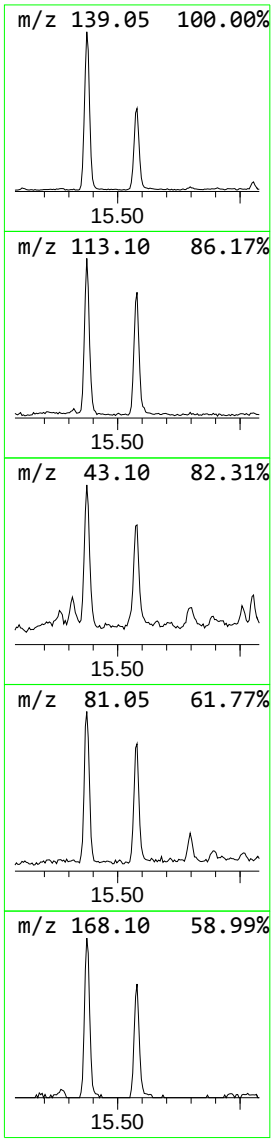
****

Peak Number 7 unknown15.579 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.579	7.85 ng	183212	Acenaphthene-d10	14.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentamethylenehydantoin	168	C8H12N2O2	000702-62-5	27
2	4-Ethyl-3-oxabicyclo[4.4.0]decane	168	C11H20O	1000216-88-3	22
3	Thiazole, 2,4-dimethyl-	113	C5H7NS	000541-58-2	22
4	4-Fluoro-N1-propyl-1,2-benzenedi...	168	C9H13FN2	300798-95-2	18
5	3,5-Heptanedione, 2,6-dimethyl-	156	C9H16O2	018362-64-6	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

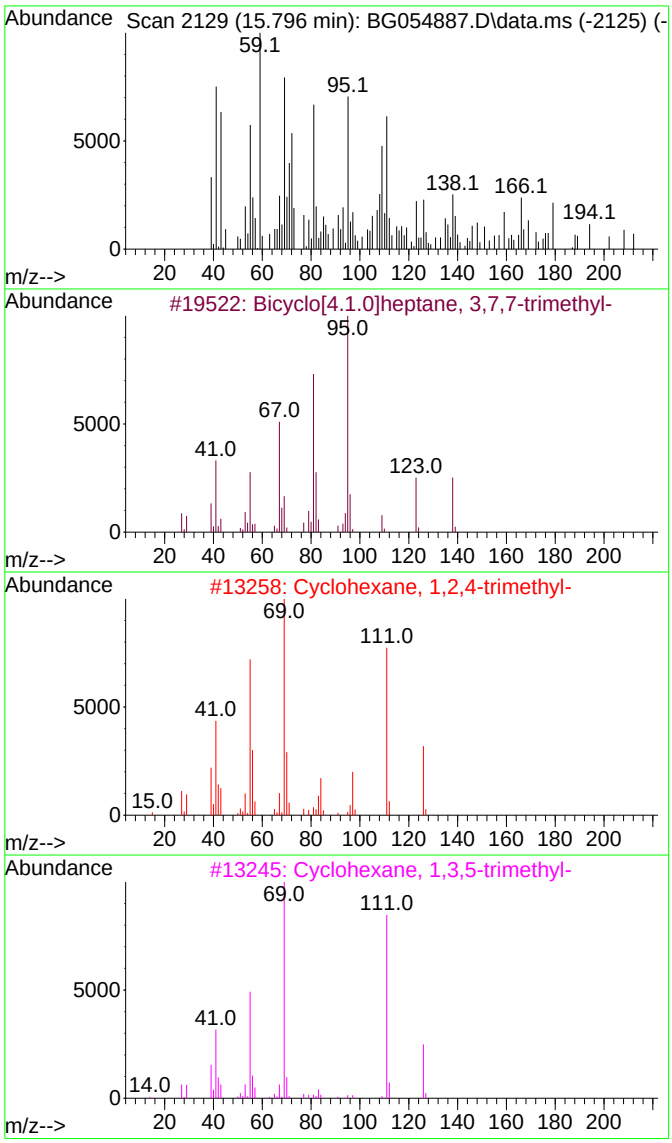
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

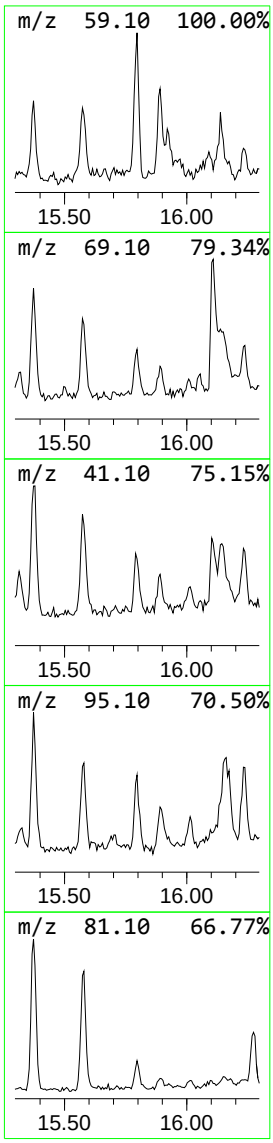
****

Peak Number 8 unknown15.796 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.796	3.10 ng	72368	Acenaphthene-d10	14.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	25
2	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	20
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	18
4	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	18
5	1,6,6-Trimethylbicyclo(3.3.0)oct...	166	C11H18O	1000427-23-1	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

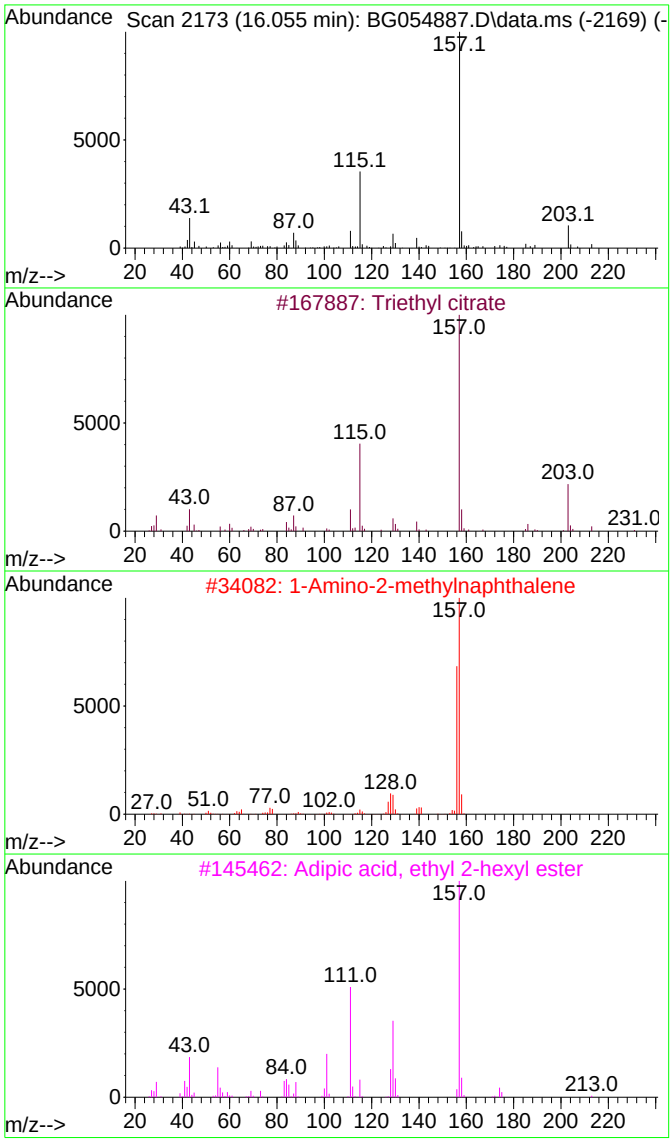
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

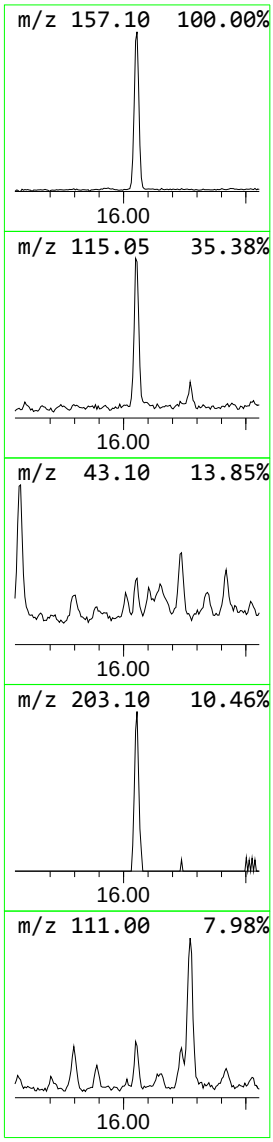
****

Peak Number 9 Triethyl citrate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.055	2.80 ng	65303	Acenaphthene-d10	14.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	78
2	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	50
3	Adipic acid, ethyl 2-hexyl ester	258	C14H26O4	1010353-70-7	40
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	33
5	Adipic acid, ethyl 3-heptyl ester	272	C15H28O4	1000353-64-6	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

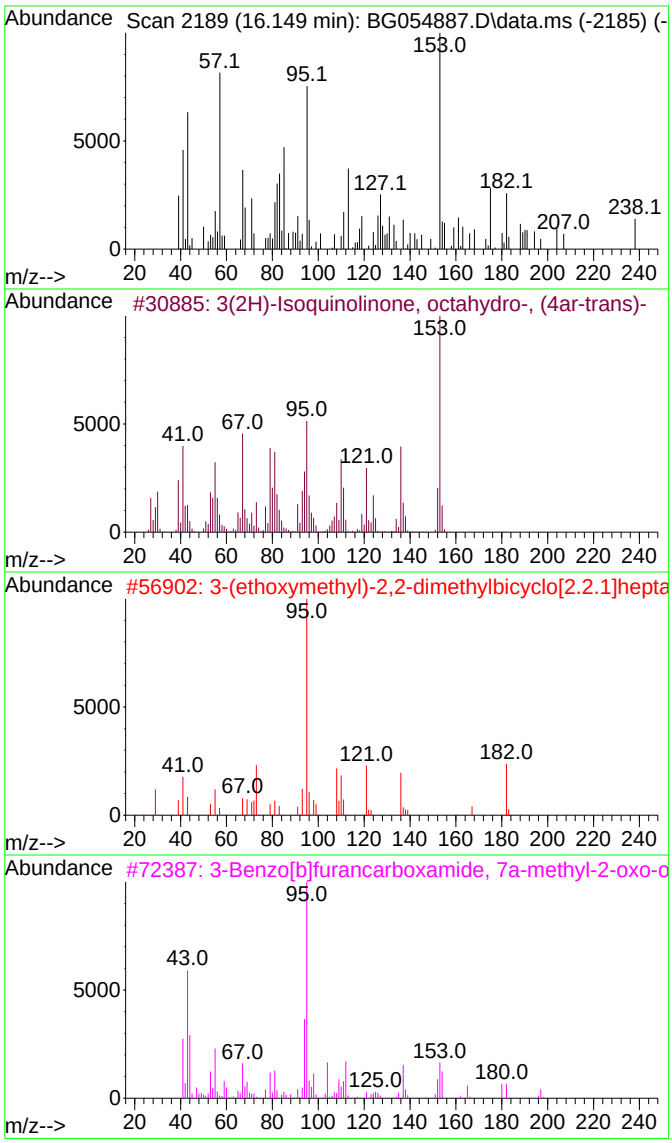
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

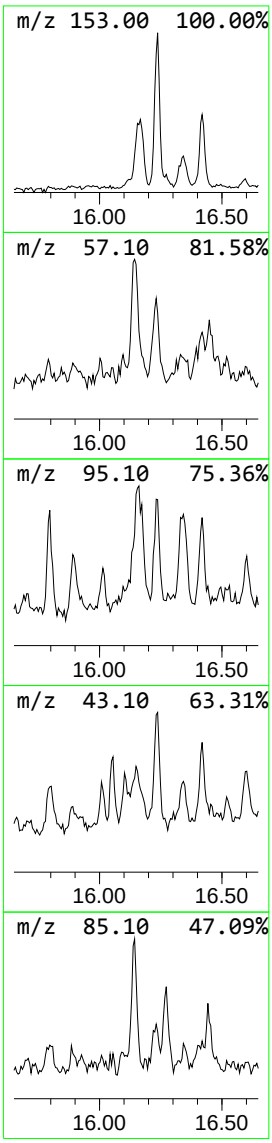
****

Peak Number 10 unknown16.149 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.149	3.90 ng	91012	Acenaphthene-d10	14.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(2H)-Isoquinolinone, octahydro-...	153	C9H15NO	076097-42-2	25
2	3-(ethoxymethyl)-2,2-dimethylbic...	182	C12H22O	1000404-89-1	14
3	3-Benzo[b]furancarboxamide, 7a-m...	197	C10H15NO3	013134-10-6	14
4	Flopropione	182	C9H10O4	002295-58-1	14
5	1-Methyl-4-ethylaminocytosine	153	C7H11N3O	092876-77-2	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

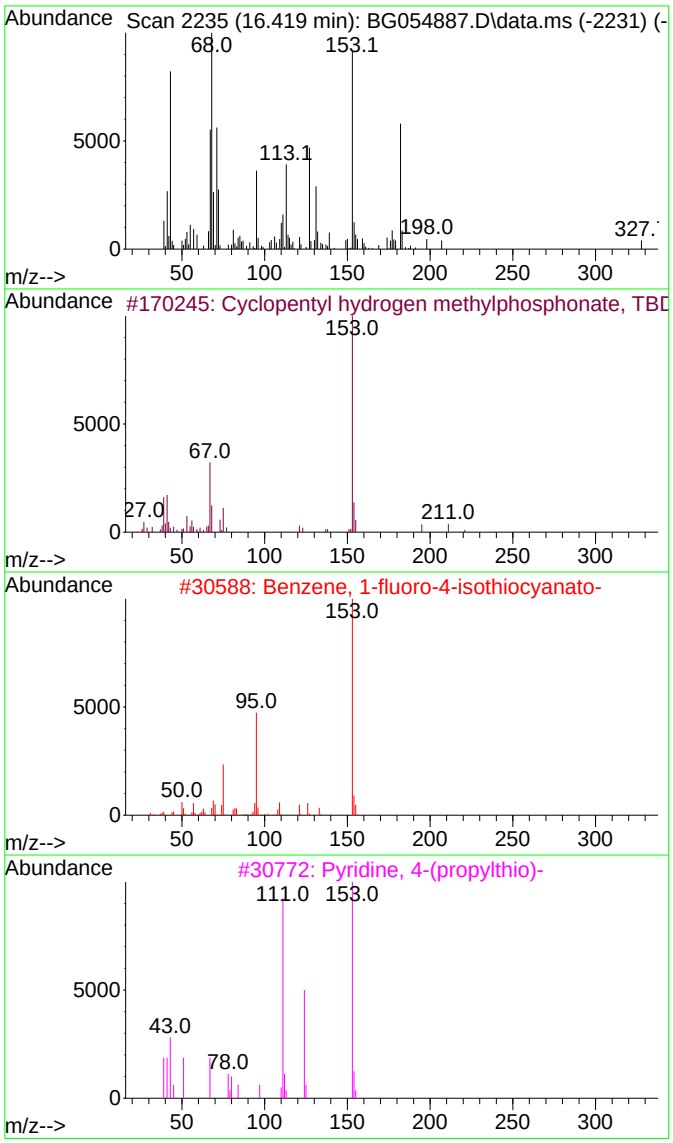
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

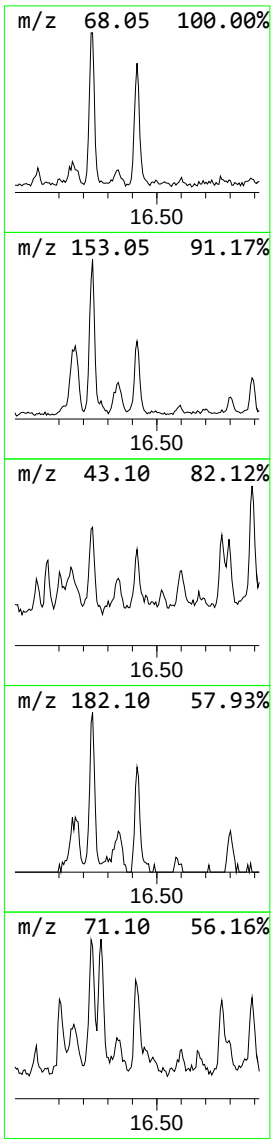
****

Peak Number 11 unknown16.419 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.419	2.64 ng	69812	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentyl hydrogen methylphosp...	278	C12H27O3PSi	1000273-46-7	14
2	Benzene, 1-fluoro-4-isothiocyanato-	153	C7H4FNS	001544-68-9	11
3	Pyridine, 4-(propylthio)-	153	C8H11NS	026891-61-2	11
4	Benzenamine, 2,4-dimethoxy-	153	C8H11NO2	002735-04-8	11
5	Ethyl 3-methylbut-3-enyl carbonate	158	C8H14O3	1000373-78-0	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

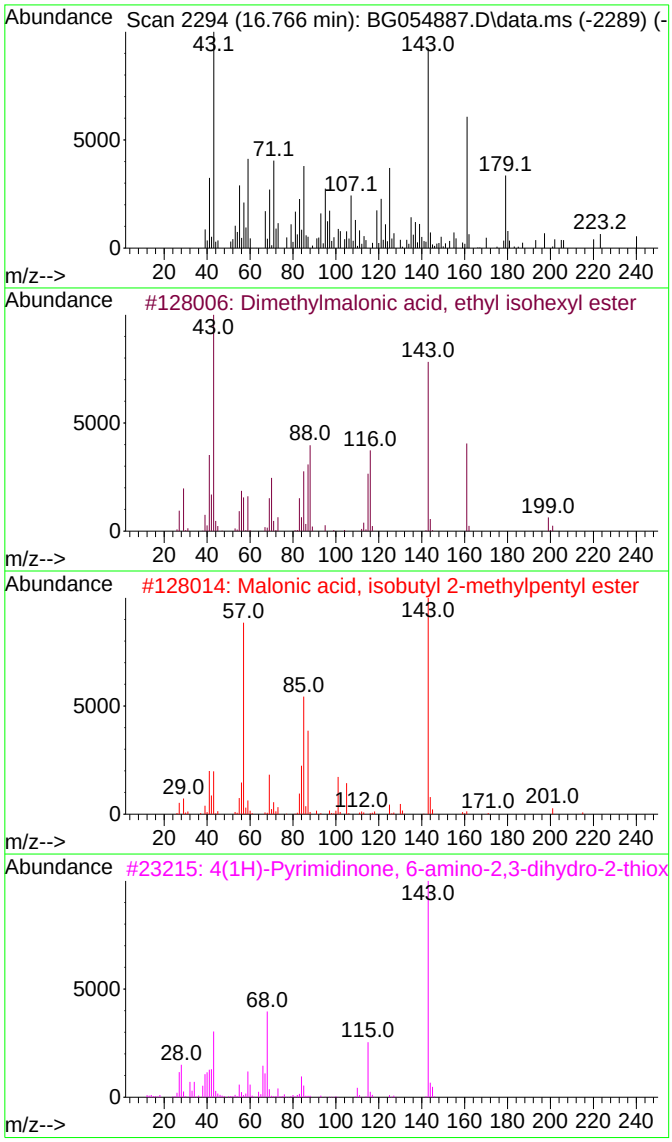
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

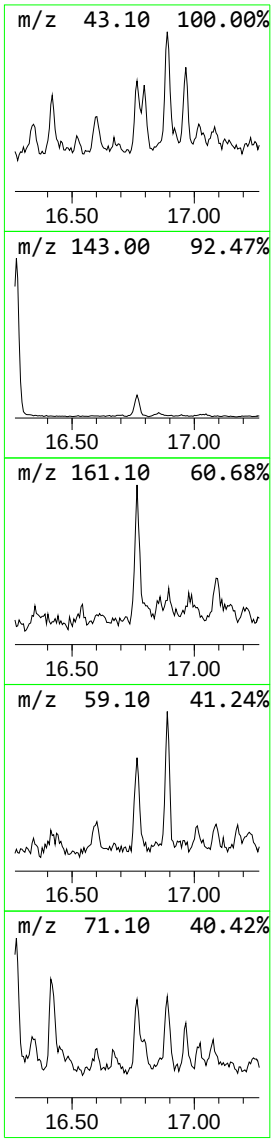
****

Peak Number 12 unknown16.766 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.766	3.09 ng	81735	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethylmalonic acid, ethyl isoh...	244	C13H24O4	1000361-71-5	32
2	Malonic acid, isobutyl 2-methylp...	244	C13H24O4	1000347-86-6	22
3	4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	14
4	Pimelic acid, di(2-propyl) ester	244	C13H24O4	1000406-56-6	14
5	N-Dodecanoyl-L-homoserine lactone	283	C16H29NO3	137173-46-7	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

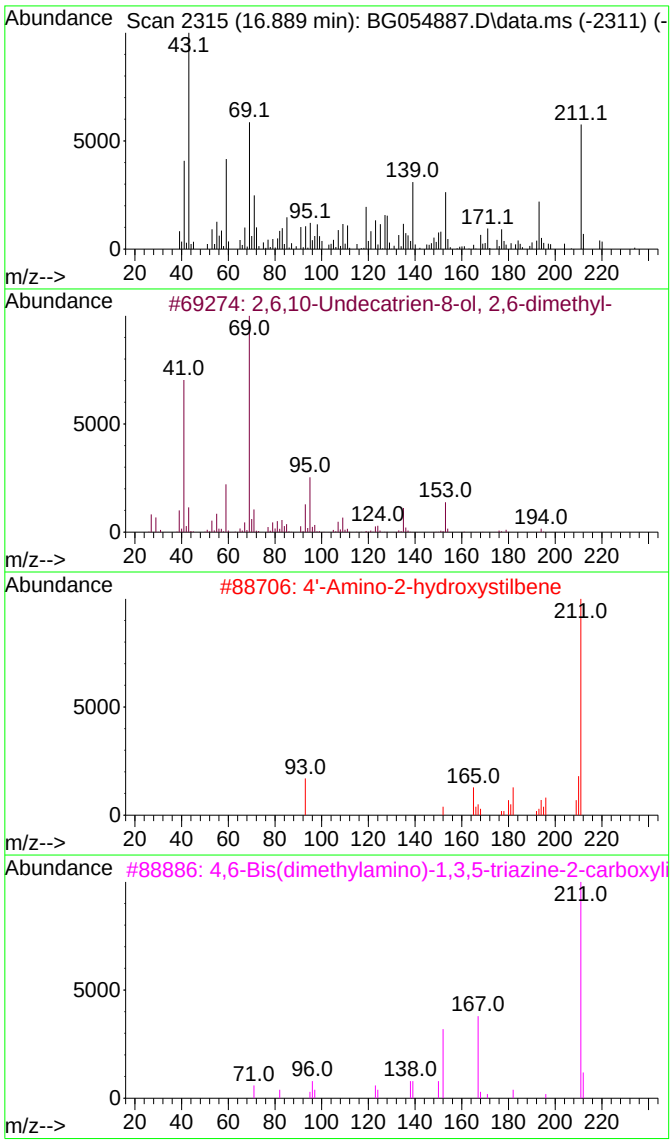
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

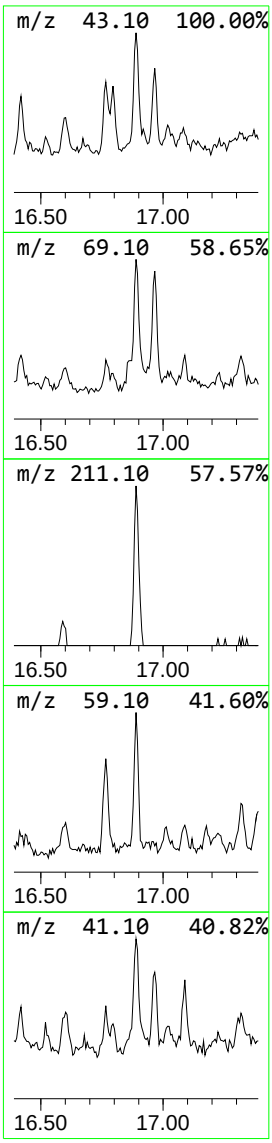
****

Peak Number 13 unknown16.889 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.889	4.16 ng	109766	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Undecatrien-8-ol, 2,6-dim...	194	C13H22O	1000163-48-4	30
2	4'-Amino-2-hydroxystilbene	211	C14H13NO	1000147-72-3	22
3	4,6-Bis(dimethylamino)-1,3,5-tri...	211	C8H13N5O2	1000101-96-9	22
4	3,4,5-Trimethoxybenzaldehyde oxime	211	C10H13NO4	039201-89-3	18
5	(Z)-4-hydroxy-3,5-dimethoxybenza...	211	C10H13NO4	1000451-81-7	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

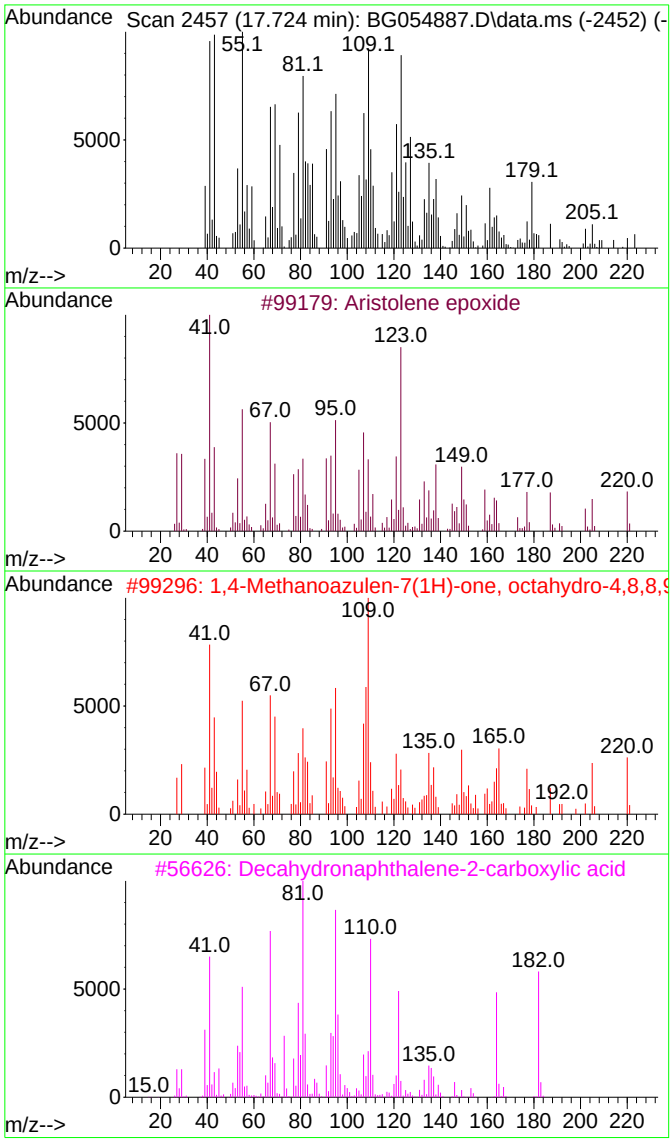
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

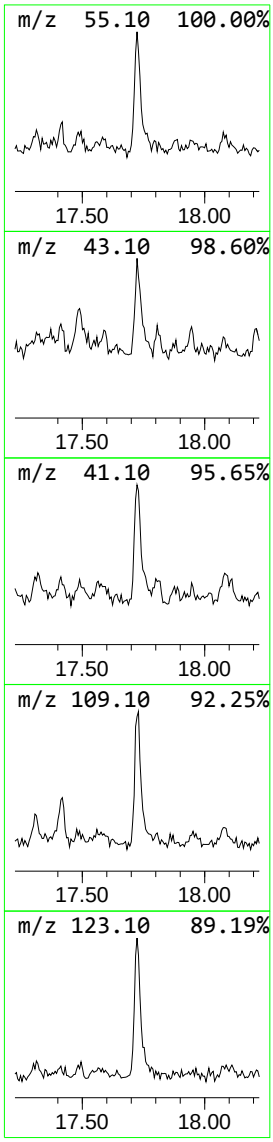
****

Peak Number 14 Aristolene epoxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.724	8.54 ng	225443	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aristolene epoxide	220	C15H24O	1000151-48-9	70
2	1,4-Methanoazulen-7(1H)-one, oct...	220	C15H24O	018319-28-3	51
3	Decahydronaphthalene-2-carboxyli...	182	C11H18O2	013032-41-2	47
4	cis-p-mentha-1(7),8-dien-2-ol	152	C10H16O	1000374-16-8	45
5	cis-Z-.alpha.-Bisabolene epoxide	220	C15H24O	1000131-71-2	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

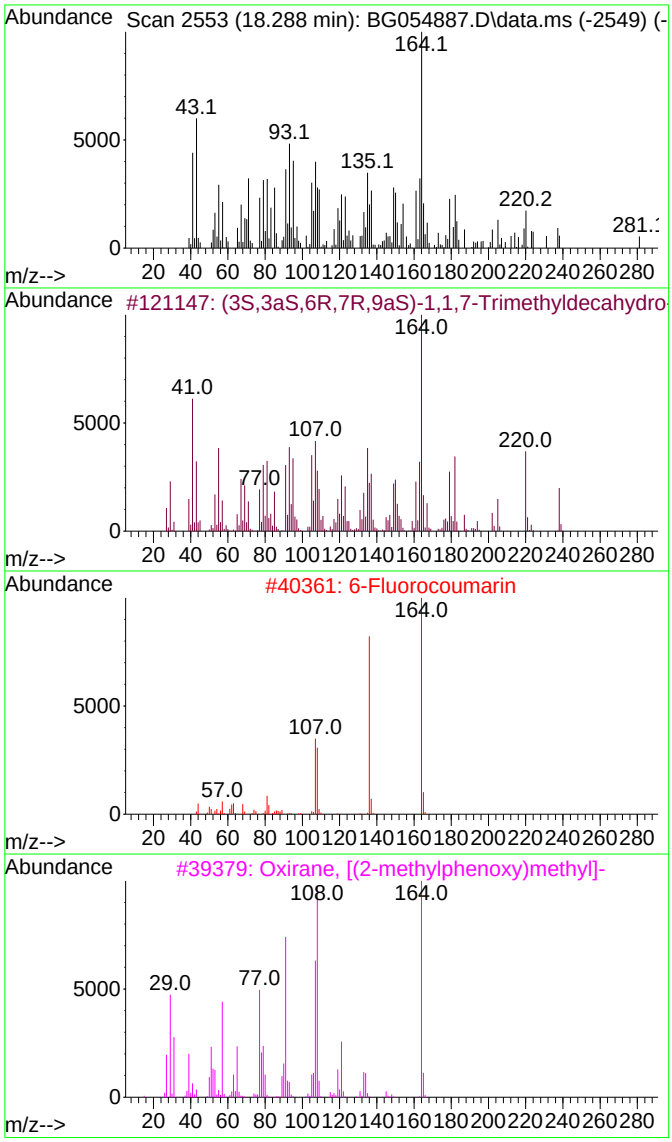
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

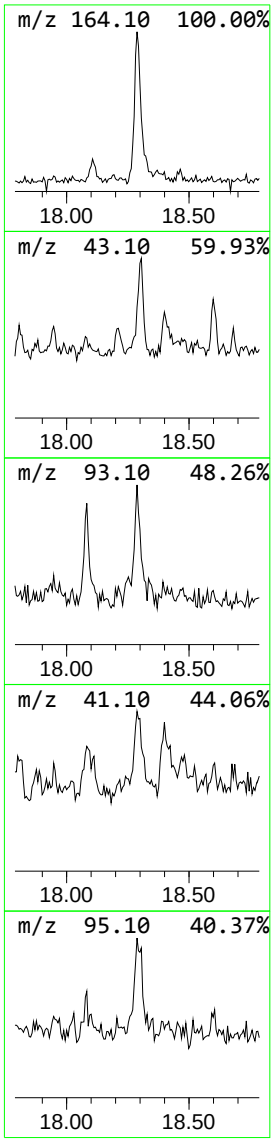
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 (3S,3aS,6R,7R,9aS)-1,1,7-Tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.288	4.15 ng	109702	Phenanthrene-d10	17.530

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,3aS,6R,7R,9aS)-1,1,7-Trimeth...	238	C15H26O2	002649-64-1	99
2	6-Fluorocoumarin	164	C9H5FO2	075487-82-0	35
3	Oxirane, [(2-methylphenoxy)methyl]-	164	C10H12O2	002210-79-9	35
4	1H-Benzimidazole, 2-(methylthio)-	164	C8H8N2S	007152-24-1	30
5	2-Propenoic acid, 3-(3-hydroxyph...	164	C9H8O3	014755-02-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

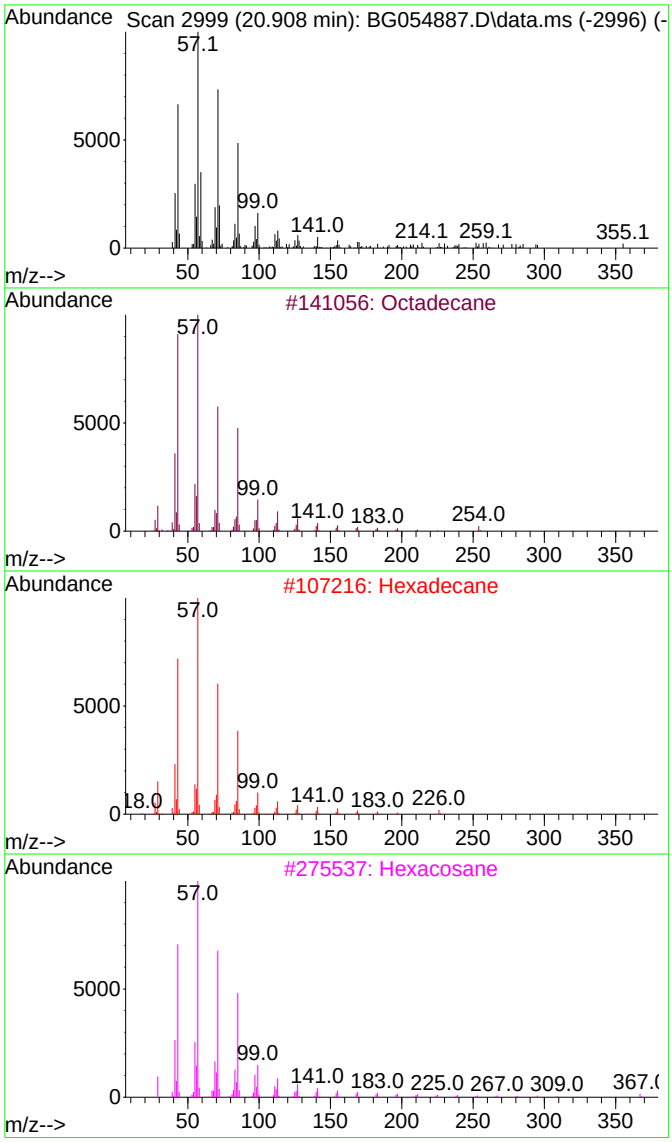
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

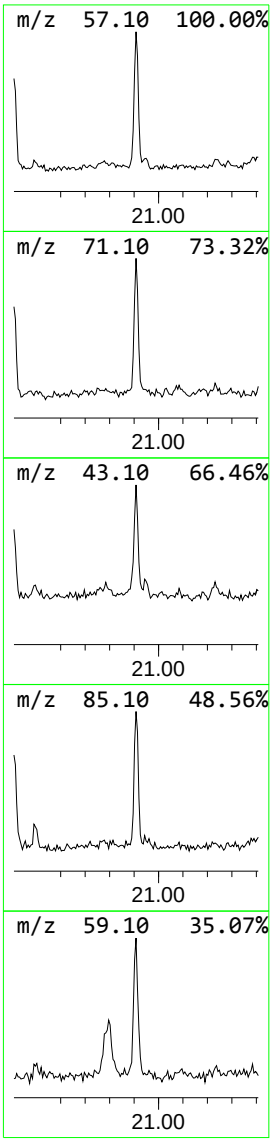
****

Peak Number 16 Octadecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.908	2.60 ng	76619	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Hexacosane	366	C26H54	000630-01-3	76
4	Octacosane	394	C28H58	000630-02-4	76
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

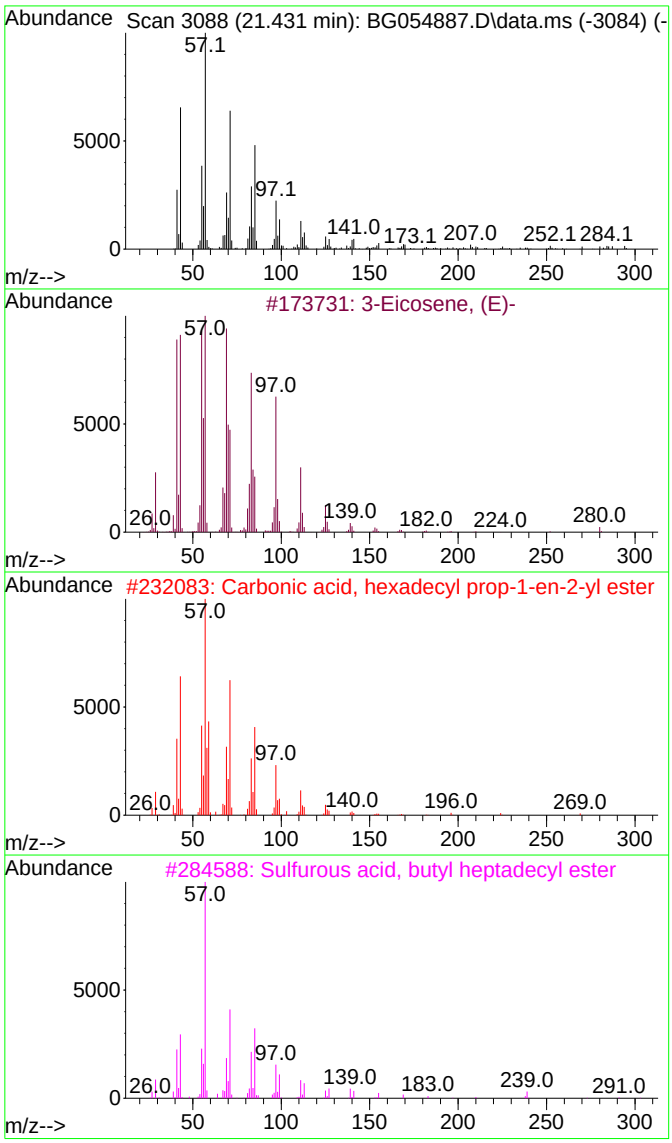
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

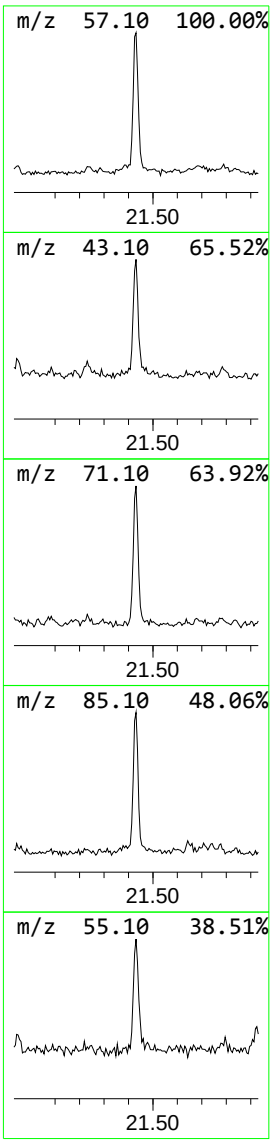
****

Peak Number 17 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.431	4.04 ng	119270	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

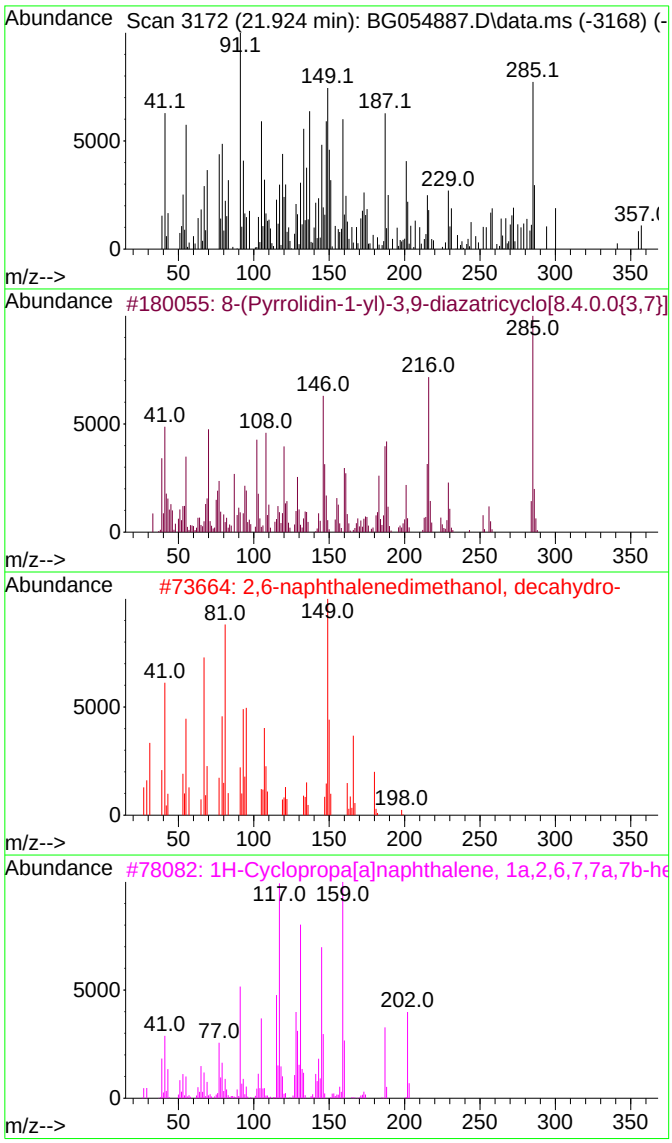
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

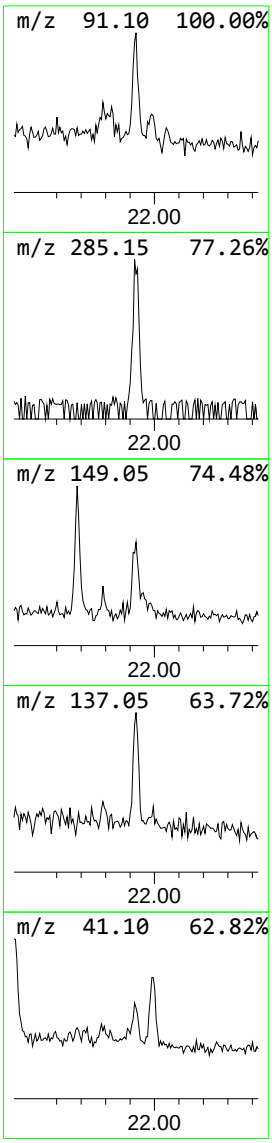
****

Peak Number 18 unknown21.924 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.924	2.92 ng	86208	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-(Pyrrolidin-1-yl)-3,9-diazatri...	285	C16H19N3S	1000435-22-5	41
2	2,6-naphthalenedimethanol, decah...	198	C12H22O2	1000400-37-5	35
3	1H-Cyclopropa[a]naphthalene, 1a,...	202	C15H22	034143-96-9	25
4	aR-Himachalene	202	C15H22	019419-67-1	25
5	4-Nitrophenol, pentafluoropropio...	285	C9H4F5NO4	959070-21-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

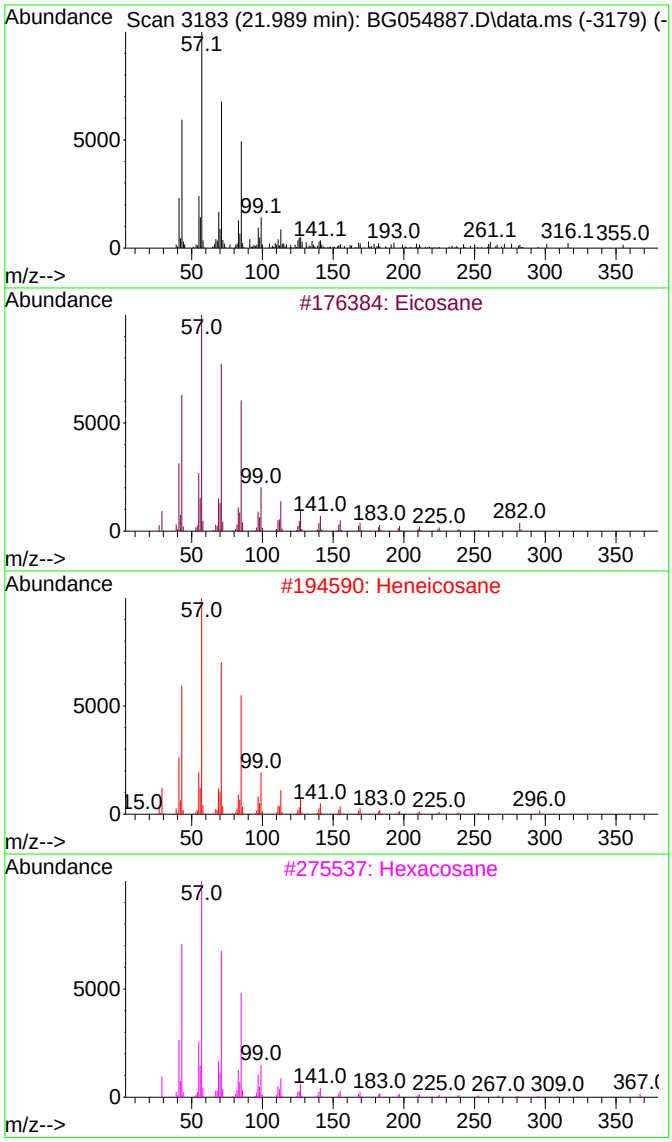
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

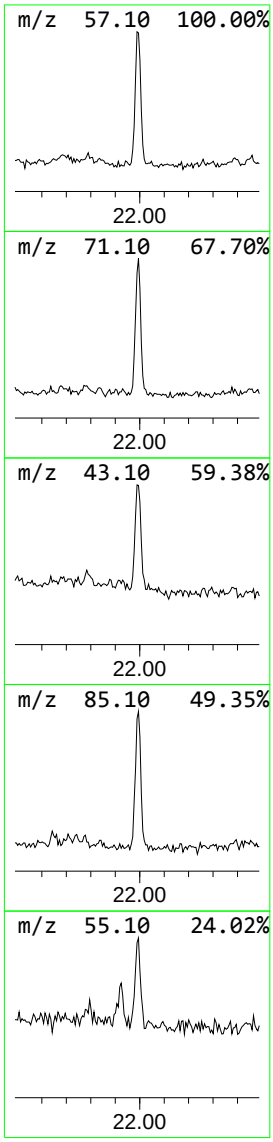
****

Peak Number 19 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.989	3.58 ng	105730	Chrysene-d12	21.831

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Pentacosane	352	C25H52	000629-99-2	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

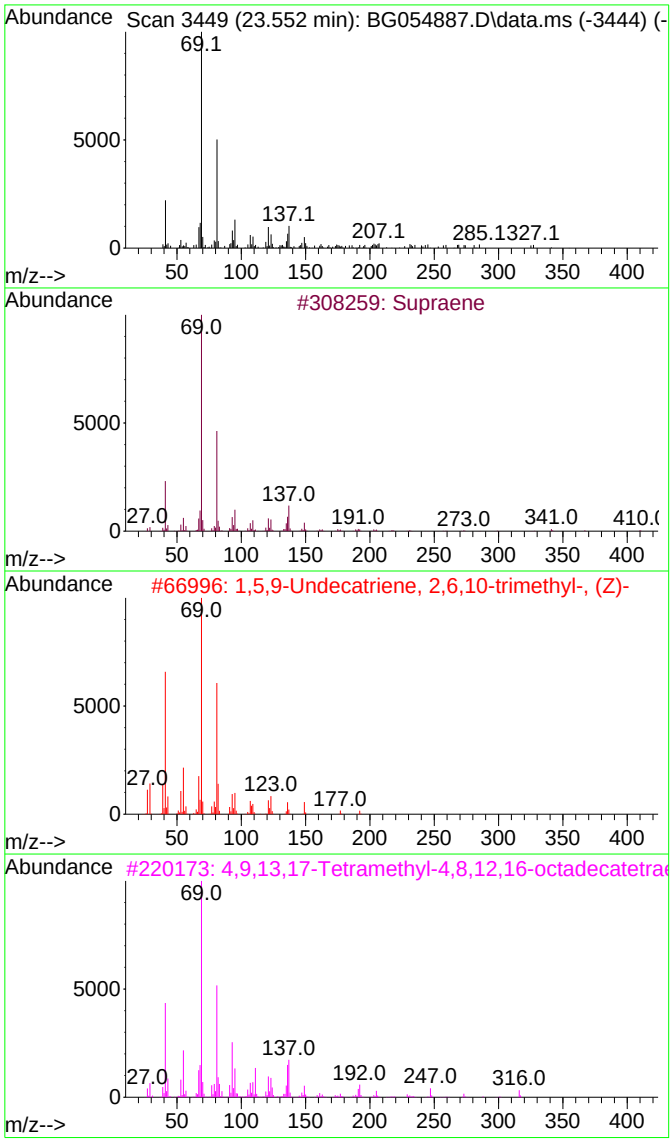
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

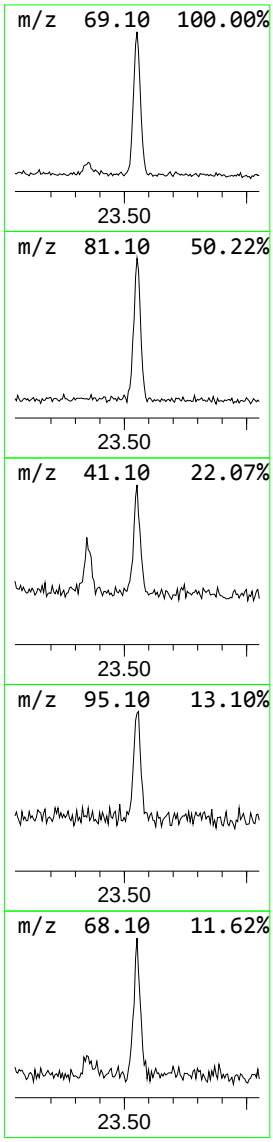
****

Peak Number 20 Supraene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.552	2.91 ng	102295	Perylene-d12	25.209

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4	3,7,11-Trimethyl-2,6,10-dodecatr...	346	C21H30O2S	1000432-39-0	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG090822\
Data File : BG054887.D
Acq On : 8 Sep 2022 17:11
Operator : CG/JU
Sample : N4537-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
Methyl Isobutyl...	3.846	2.9	ng	27576	1	8.147	192262	20.0
2-Pentanone, 4-...	5.203	4.1	ng	39709	1	8.147	192262	20.0
Ethanol, 2-(2-b...	10.726	2.7	ng	38288	2	10.973	287983	20.0
unknown12.794	12.794	2.8	ng	40500	2	10.973	287983	20.0
1,3-Dimethyl-3,...	14.416	5.4	ng	125656	3	14.786	466767	20.0
unknown15.373	15.373	10.9	ng	254558	3	14.786	466767	20.0
unknown15.579	15.579	7.8	ng	183212	3	14.786	466767	20.0
unknown15.796	15.796	3.1	ng	72368	3	14.786	466767	20.0
Triethyl citrate	16.055	2.8	ng	65303	3	14.786	466767	20.0
unknown16.149	16.149	3.9	ng	91012	3	14.786	466767	20.0
unknown16.419	16.419	2.6	ng	69812	4	17.530	528239	20.0
unknown16.766	16.766	3.1	ng	81735	4	17.530	528239	20.0
unknown16.889	16.889	4.2	ng	109766	4	17.530	528239	20.0
Aristolene epoxide	17.724	8.5	ng	225443	4	17.530	528239	20.0
(3S,3aS,6R,7R,9...	18.288	4.2	ng	109702	4	17.530	528239	20.0
Octadecane	20.908	2.6	ng	76619	5	21.831	590391	20.0
3-Eicosene, (E)-	21.431	4.0	ng	119270	5	21.831	590391	20.0
unknown21.924	21.924	2.9	ng	86208	5	21.831	590391	20.0
Eicosane	21.989	3.6	ng	105730	5	21.831	590391	20.0
Supraene	23.552	2.9	ng	102295	6	25.209	702124	20.0