LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

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_M\Methods\8270-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.763	259	268	280	rBV	63569	153383	2.14%	0.273%
2	5.010	306	310	319	rVB	151851	206293	2.87%	0.367%
3	5.463	380	387	398	rBV	1165168	1685582	23.49%	2.998%
4	5.875	449	457	465	rBV	199892	298439	4.16%	0.531%
5	7.093	656	664	673	rBV	1136898	1842094	25.67%	3.277%
6	7.922	797	805	818	rBV	407218	683602	9.53%	1.216%
7	8.187	844	850	862	rBV	96350	188431	2.63%	0.335%
8	9.122	1002	1009	1016	rBV	726189	1146875	15.98%	2.040%
9	10.739	1277	1284	1290	rBV	455795	744694	10.38%	1.325%
10	12.151	1518	1524	1534	rVV4	43214	107751	1.50%	0.192%
11	12.375	1554	1562	1584	rBV3	39029	149852	2.09%	0.267%
12	12.569	1588	1595	1609	rBV	252425	712527	9.93%	1.267%
13	13.192	1695	1701	1709	rVB	1356560	1885994	26.28%	3.355%
14	14.039	1839	1845	1855	rVB	888431	1168222	16.28%	2.078%
15	14.186	1863	1870	1880	rBV	176030	307616	4.29%	0.547%
16	14.304	1884	1890	1894	rBV	65845	101412	1.41%	0.180%
17	14.569	1927	1935	1942	rBV	636097	989650	13.79%	1.760%
18	14.639	1942	1947	1955	rVB2	61577	120903	1.68%	0.215%
19	14.957	1993	2001	2008	rBV3	34643	77071	1.07%	0.137%
20	15.310	2055	2061	2072	rBV	529607	714180	9.95%	1.270%
21	15.616	2108	2113	2121	rVB2	46798	80944	1.13%	0.144%
22	16.063	2183	2189	2199	rVB	1256966	1774346	24.72%	3.156%
23	16.310	2227	2231	2236	rVB	57067	94384	1.32%	0.168%
24	16.427	2248	2251	2257	rVB3	61863	103213	1.44%	0.184%
25	16.686	2290	2295	2300	rBV4	177594	262066	3.65%	0.466%
26	17.063	2354	2359	2365	rBV	267785	327788	4.57%	0.583%
27	17.121	2365	2369	2374	rVV2	79159	159227	2.22%	0.283%
28	17.174	2374	2378	2386	rVB2	200672	290563	4.05%	0.517%
29	17.239	2386	2389	2394	rBV	99835	123842	1.73%	0.220%
30	17.321	2399	2403	2407	rVV	735263	1048943	14.62%	1.866%
31	17.363	2407	2410	2418	rVB	783543	1090520	15.20%	1.940%
32	17.457	2421	2426	2432	rVB	210977	323060	4.50%	0.575%
33	17.745	2472	2475	2481	rVB	103705	144908	2.02%	0.258%
34	18.063	2523	2529	2535	rBV3	165779	371225	5.17%	0.660%
35	18.121	2536	2539	2544	rBV2	77814	115543	1.61%	0.206%
36	18.192	2544	2551	2557	rBV	4582044	7176709	100.00%	12.766%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

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_M\Methods\8270-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.392	2581	2585	2589	rBV3	117976	189969	2.65%	0.338%
38	18.757	2644	2647	2655	rVB2	147174	216270	3.01%	0.385%
39	18.845	2659	2662	2666	rBV2	156445	205170	2.86%	0.365%
40	19.033	2691	2694	2698	rVB3	127387	143945	2.01%	0.256%
41	19.339	2744	2746	2748	rBV	165207	175880	2.45%	0.313%
42	19.380	2748	2753	2758	rVB	2282941	3086890	43.01%	5.491%
43	19.462	2759	2767	2776	rBV2	2791907	4259033	59.35%	7.576%
44	19.704	2805	2808	2811	rBV3	272622	403066	5.62%	0.717%
45	19.745	2811	2815	2823	rVB2	1785259	2711174	37.78%	4.823%
46	19.939	2844	2848	2855	rVB	2045465	2441728	34.02%	4.343%
47	21.374	3089	3092	3100	rBV3	802200	1197434	16.69%	2.130%
48	21.503	3108	3114	3118	rBV2	1091979	2436629	33.95%	4.334%
49	21.545	3118	3121	3125	rVB	894152	1029092	14.34%	1.831%
50	22.050	3204	3207	3211	rBV	501588	565859	7.88%	1.007%
51	23.086	3379	3383	3392	rVB	965361	1541692	21.48%	2.742%
52	23.180	3393	3399	3405	rBV2	876640	2331562	32.49%	4.147%
53	23.715	3486	3490	3501	rVB	549065	1150764	16.03%	2.047%
54	23.821	3503	3508	3516	rVB	653279	1272698	17.73%	2.264%
55	23.933	3522	3527	3532	rBV	461074	832894	11.61%	1.482%
56	24.415	3605	3609	3619	rVB	410085	862138	12.01%	1.534%
57	27.262	4086	4093	4111	rVB4	693649	2393430	33.35%	4.257%

Sum of corrected areas: 56219169

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
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Acq On : 31 Oct 2023 20:10
Operator : MA/JU
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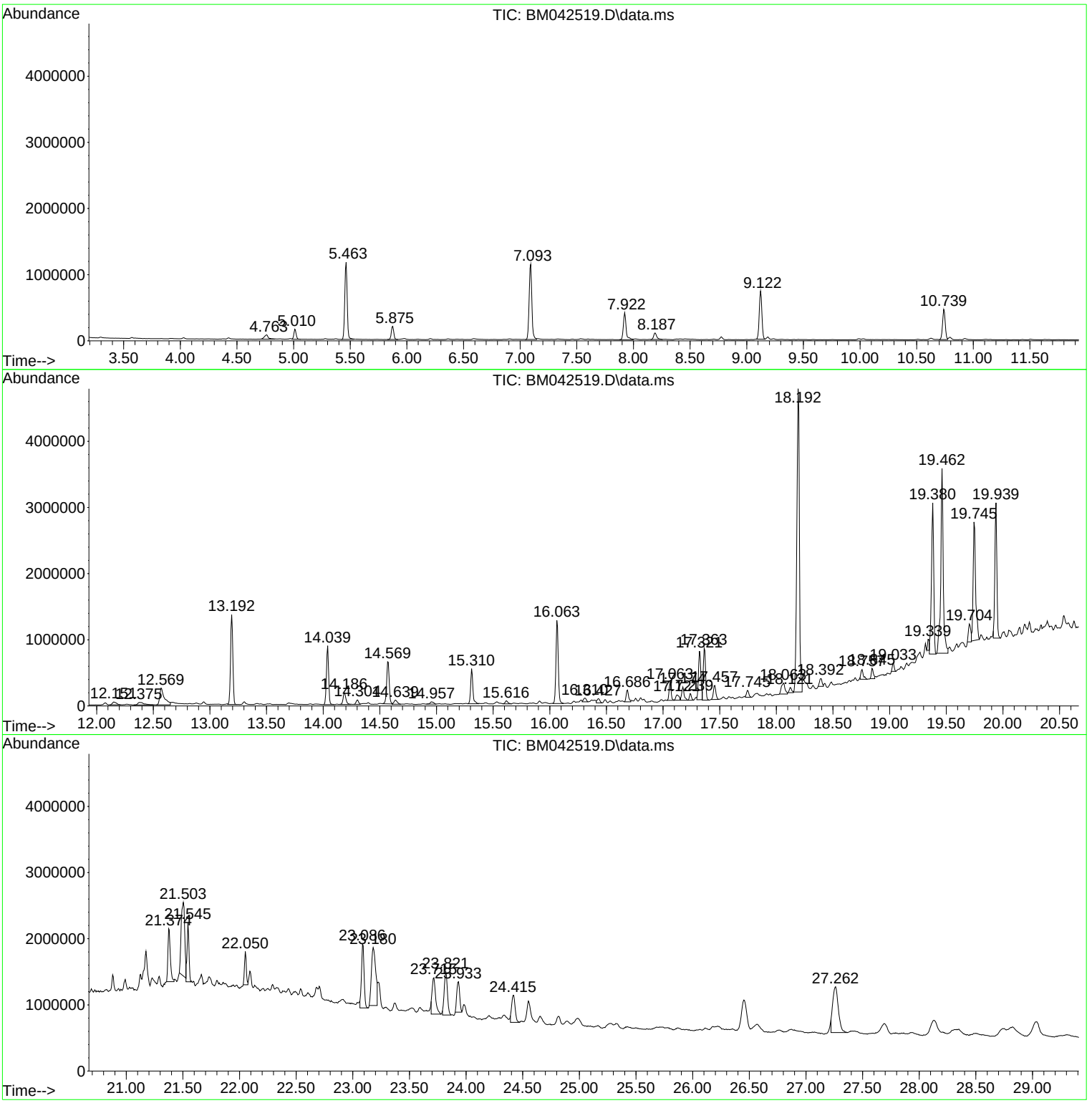
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

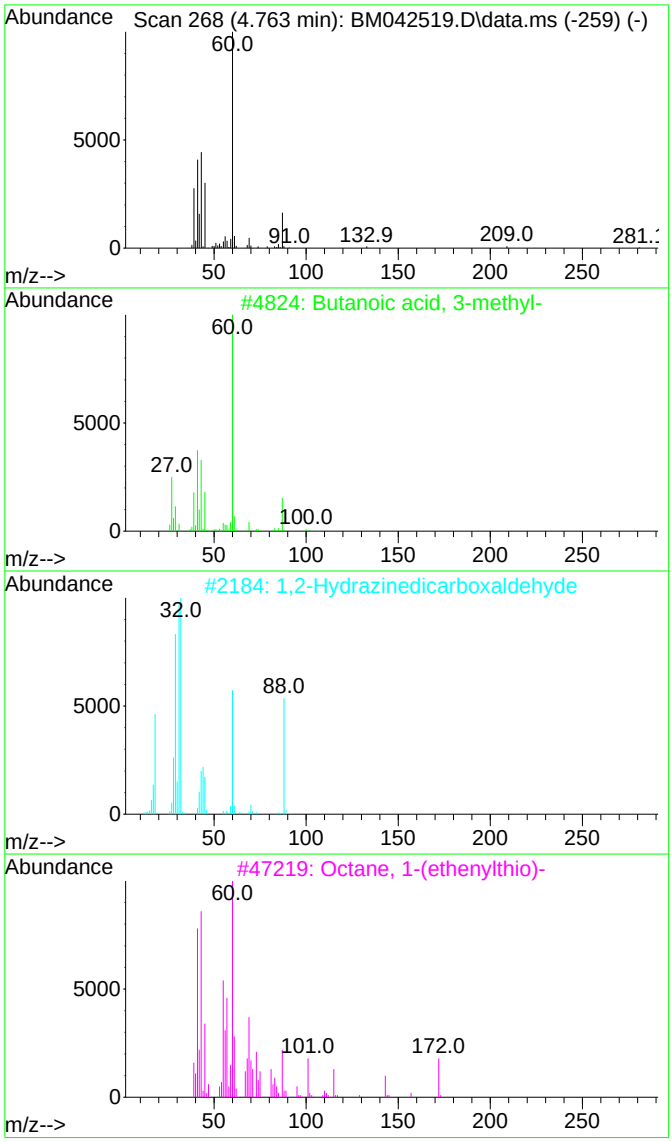
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

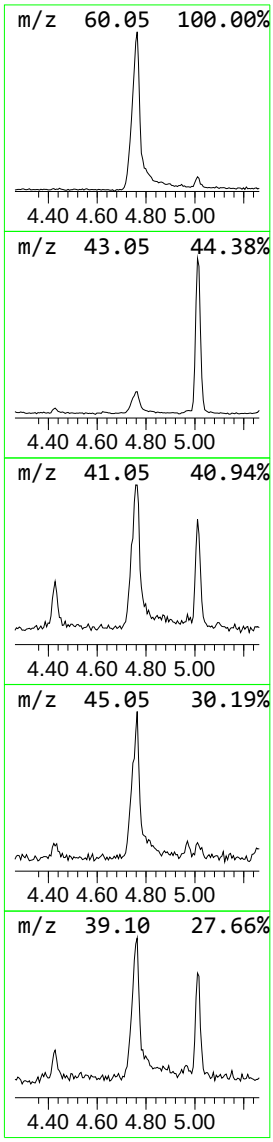
****

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.763	4.49 ng	153383	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	40
3	Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	40
4	N-Carbomethoxy-N-methoxymethylamine	119	C4H9NO3	153654-07-0	39
5	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

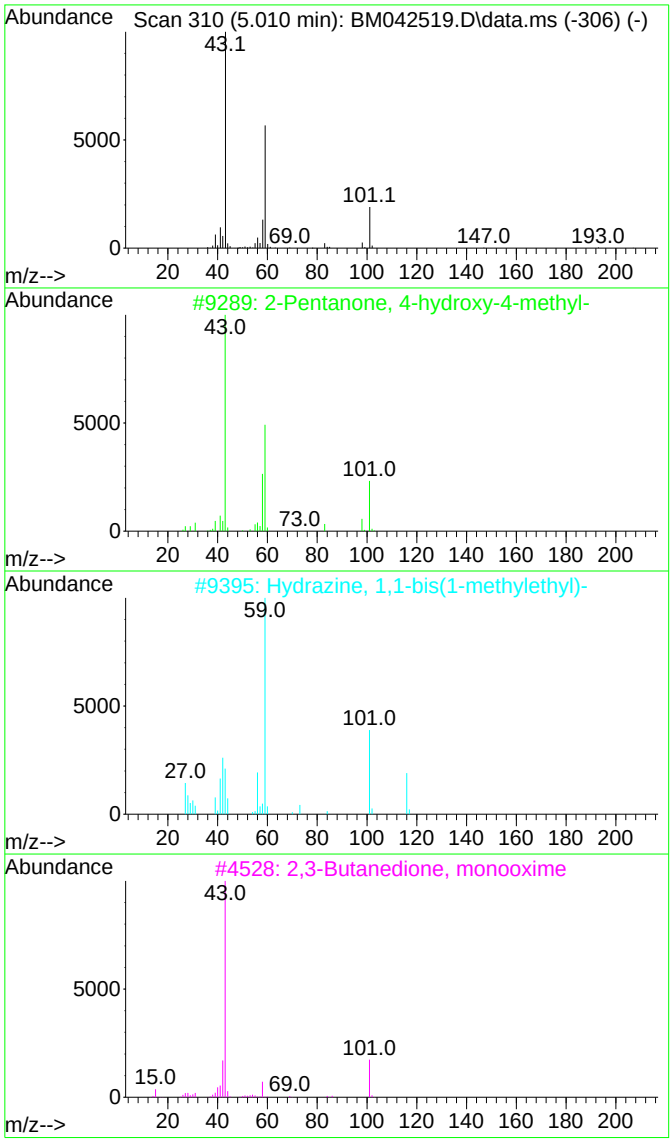
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

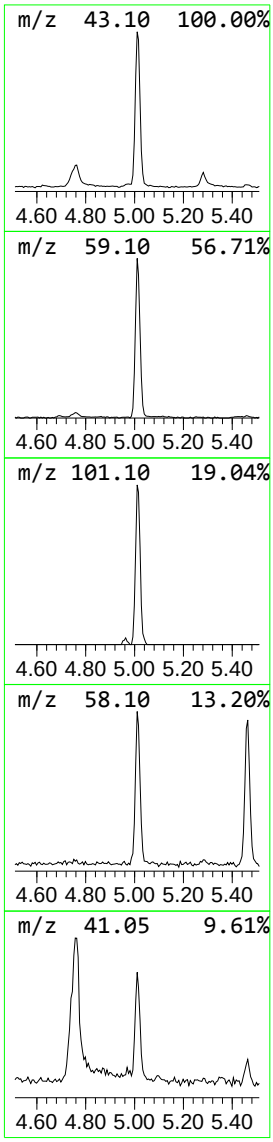
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	6.04 ng	206293	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

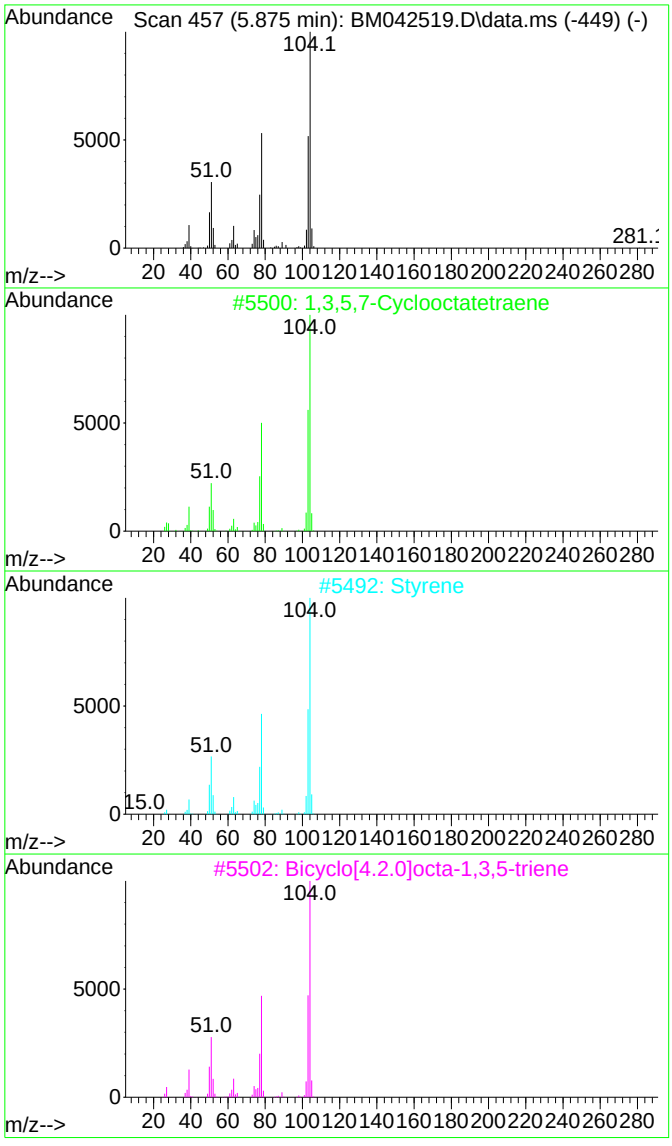
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

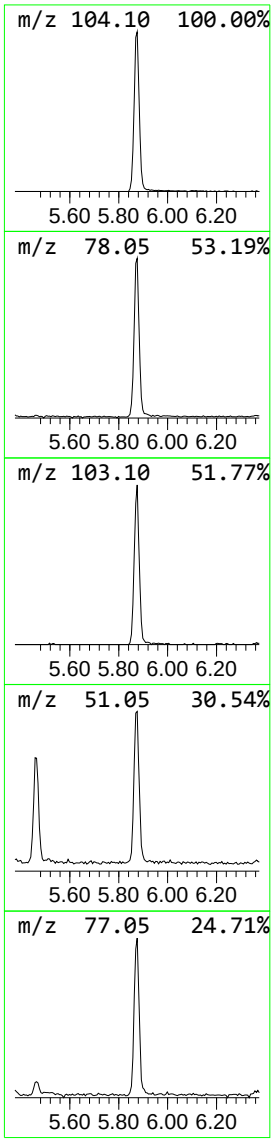
****

Peak Number 3 1,3,5,7-Cyclooctatetraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	8.73 ng	298439	1,4-Dichlorobenzene-d4	7.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	97
2	Styrene	104	C8H8	000100-42-5	96
3	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	94
4	Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	72
5	2-Pyridinecarbonitrile	104	C6H4N2	000100-70-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

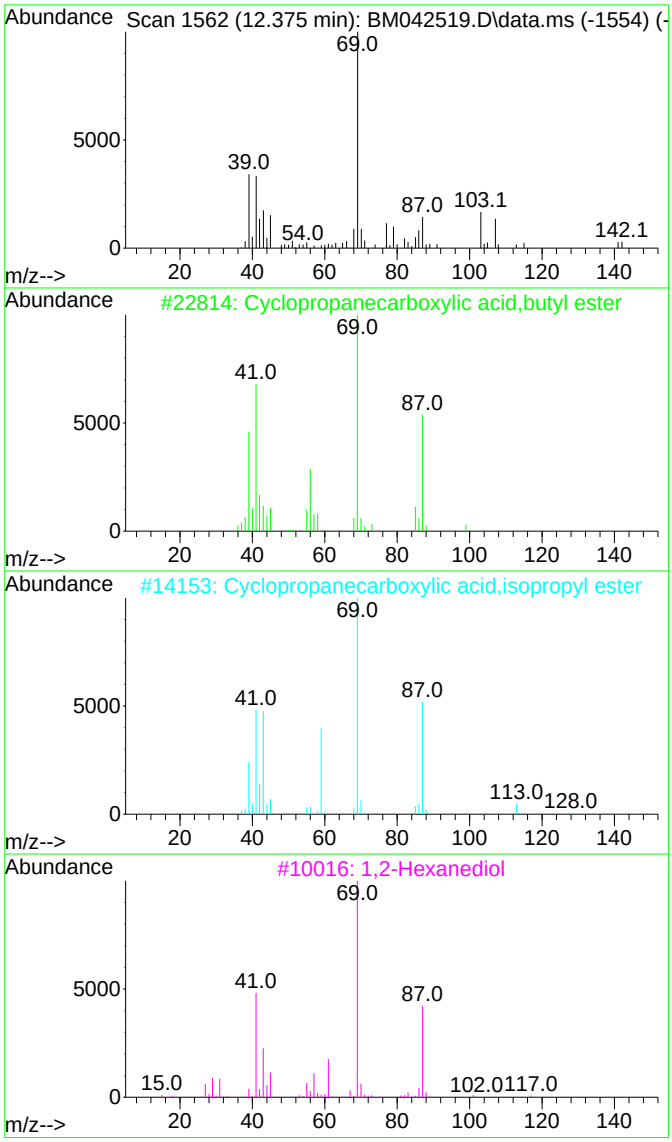
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

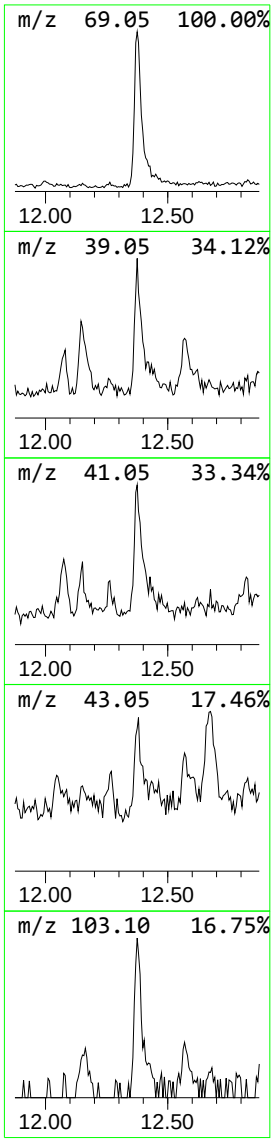
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropanecarboxylic acid... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.375	4.02 ng	149852	Naphthalene-d8	10.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid,buty...	142	C8H14O2	054947-39-6	50
2	Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	38
3	1,2-Hexanediol	118	C6H14O2	006920-22-5	38
4	4,5-Octanediol, 2,7-dimethyl-	174	C10H22O2	1000153-20-8	33
5	2-Propenoic acid, 2-methyl-, 3-m...	156	C9H16O2	007336-27-8	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

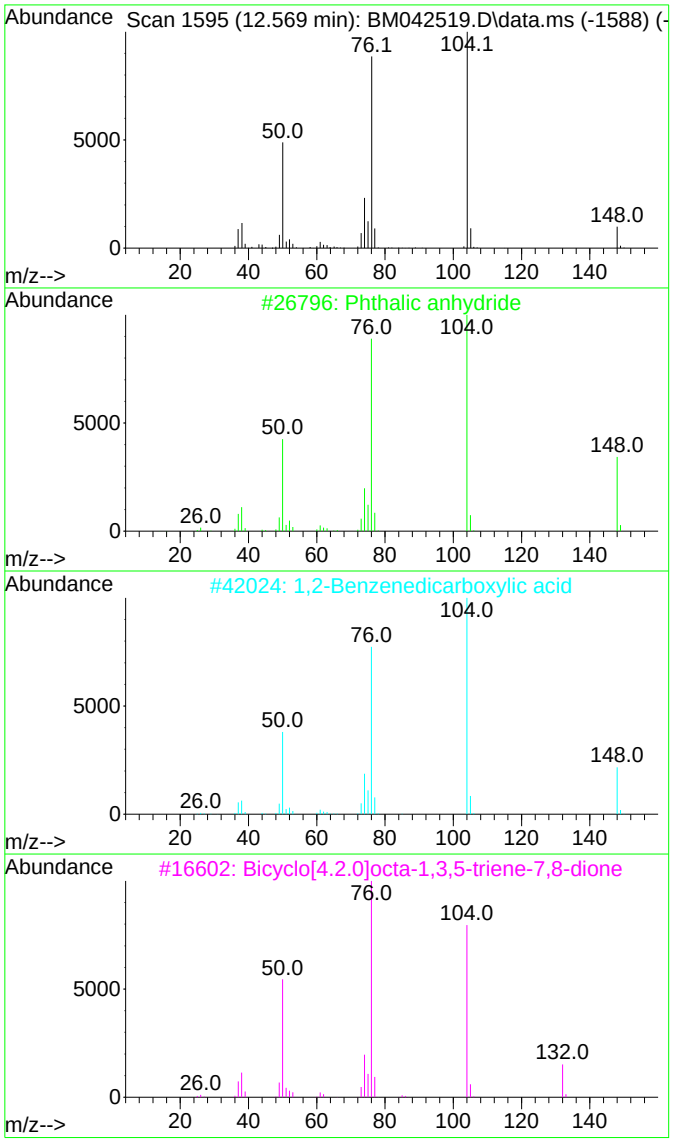
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

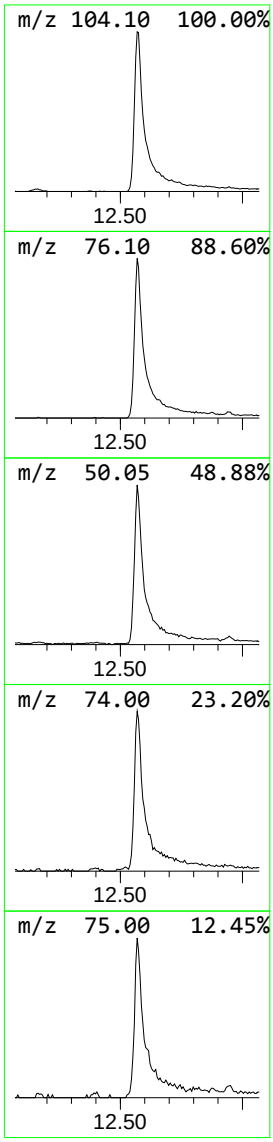
****

Peak Number 5 Phthalic anhydride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	19.14 ng	712527	Naphthalene-d8	10.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	96
2	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	91
3	Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	91
4	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	83
5	Methyl hydrogen phthalate	180	C9H8O4	004376-18-5	78





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Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

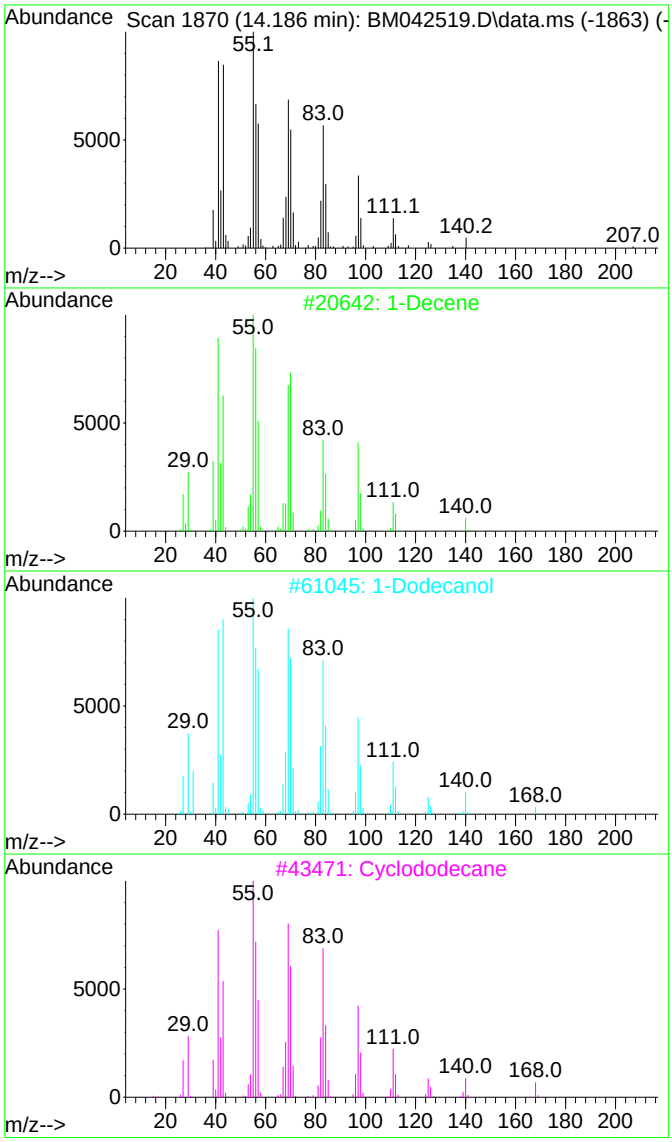
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

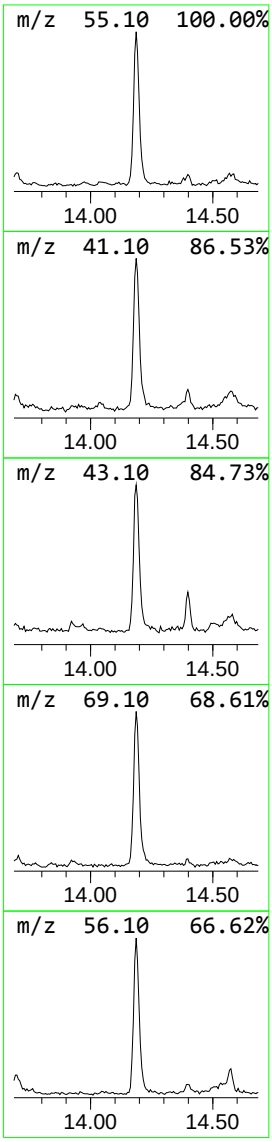
****

Peak Number 6 1-Decene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.186	6.22 ng	307616	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene	140	C10H20	000872-05-9	96
2	1-Dodecanol	186	C12H26O	000112-53-8	91
3	Cyclododecane	168	C12H24	000294-62-2	91
4	Cyclodecane	140	C10H20	000293-96-9	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

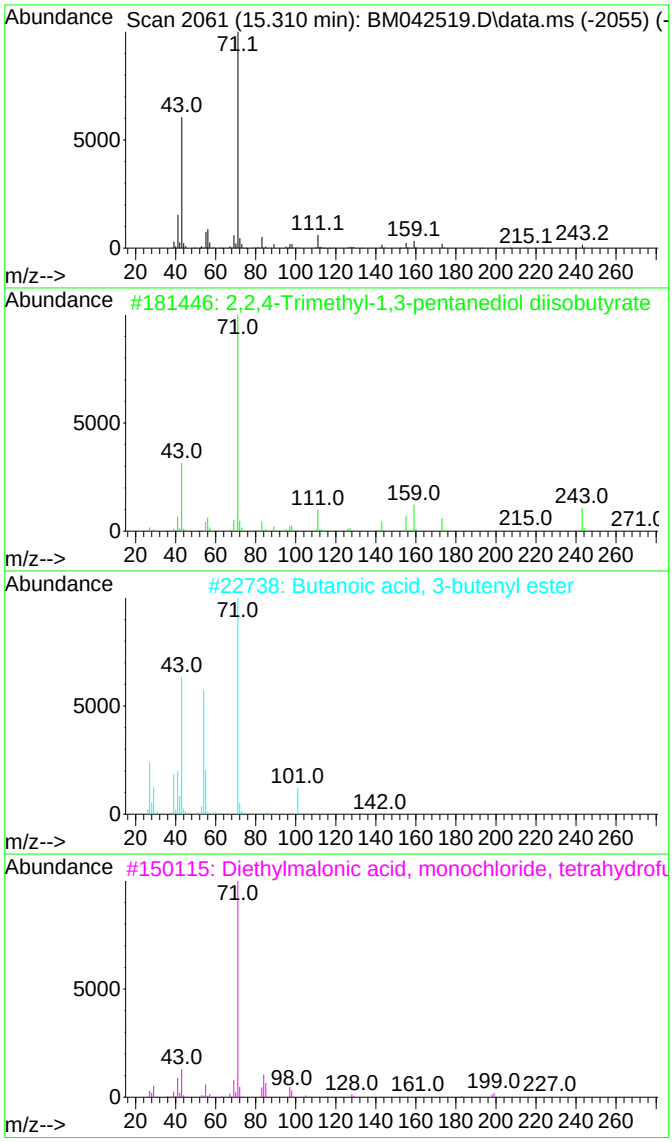
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

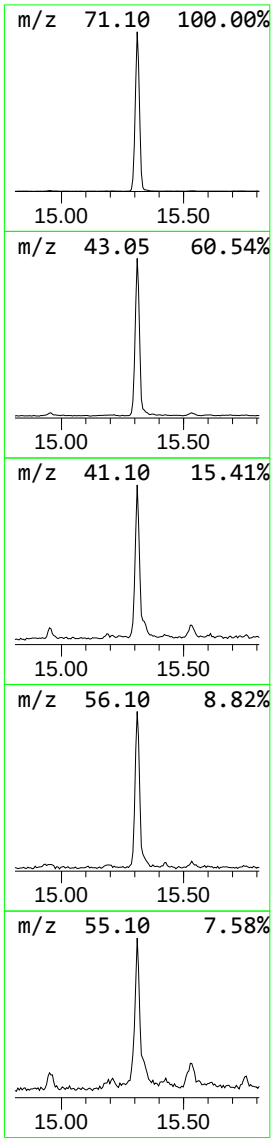
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	14.43 ng	714180	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83
2	Butanoic acid, 3-butenyl ester	142	C8H14O2	021698-32-8	64
3	Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	64
4	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	50
5	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
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Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

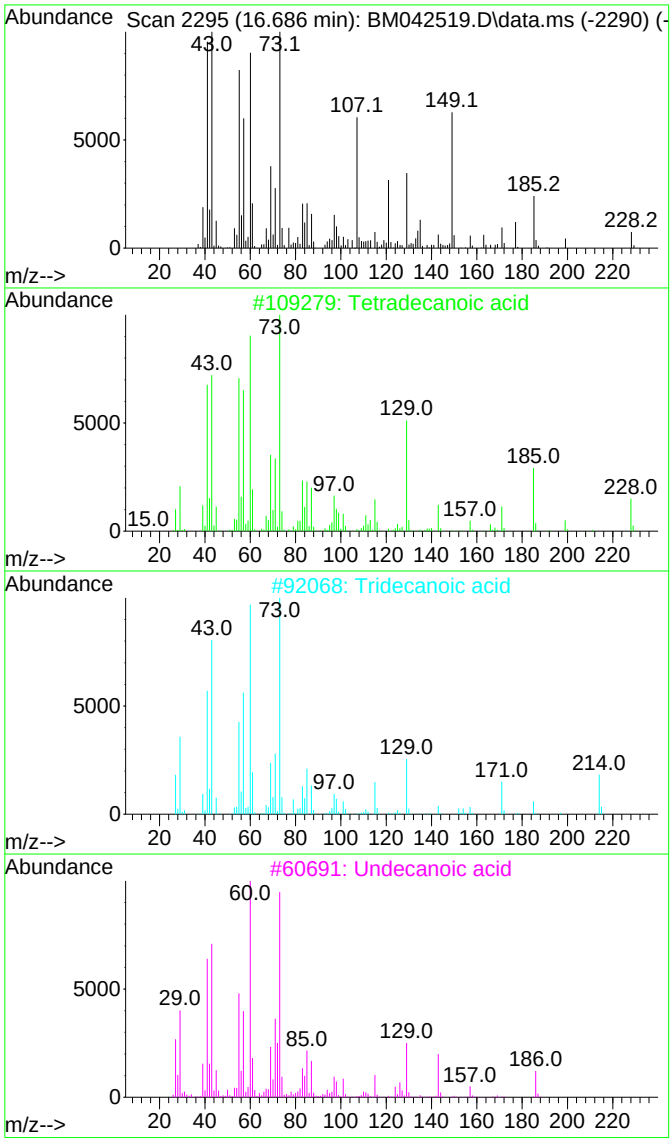
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

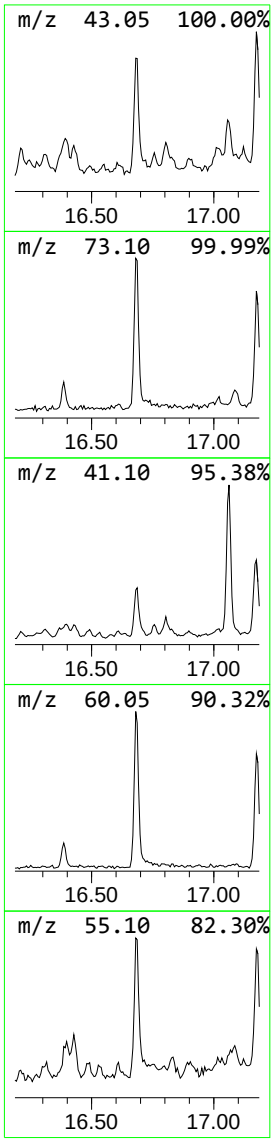
****

Peak Number 8 Tetradecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.686	5.00 ng	262066	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	49
3	Undecanoic acid	186	C11H22O2	000112-37-8	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	38
5	Octanoic acid	144	C8H16O2	000124-07-2	38





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Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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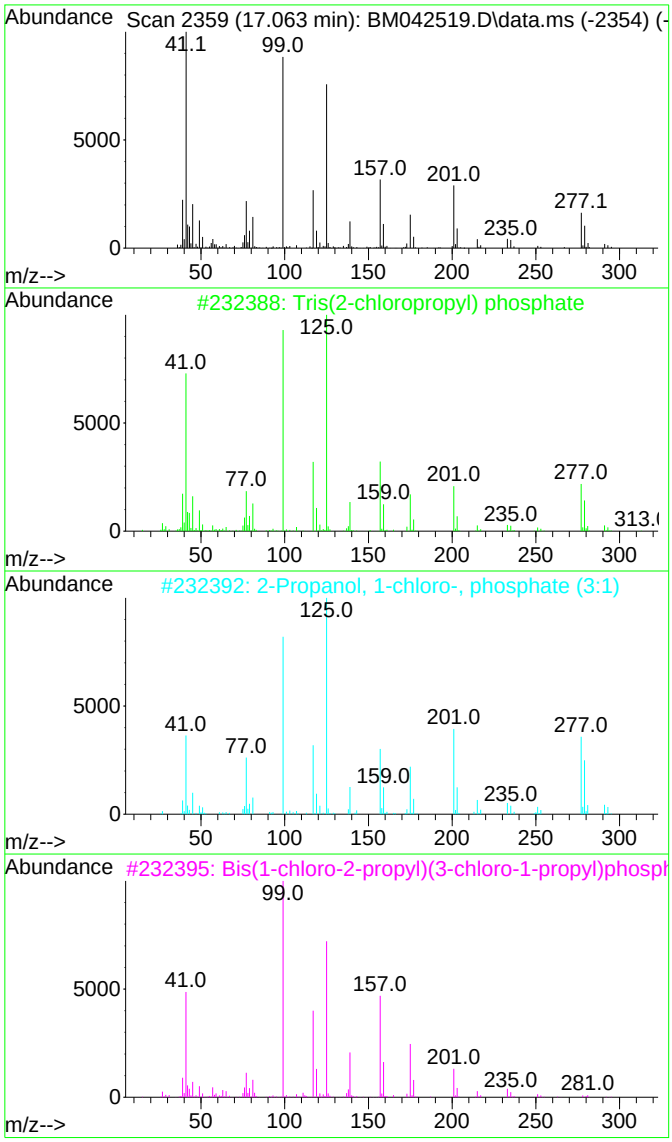
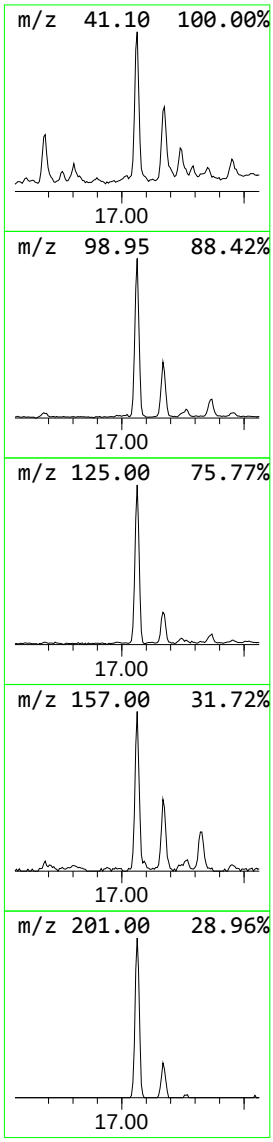
Peak Number 9 Tris(2-chloropropyl) phosphate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.063	6.25 ng	327788	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tris(2-chloropropyl) phosphate	326	C9H18Cl3O4P	006145-73-9	91
2	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	45
3	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	43
4	Sarin	140	C4H10FO2P	000107-44-8	28
5	Bis(3-chloro-1-propyl)(1-chloro-...	326	C9H18Cl3O4P	137888-35-8	16





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Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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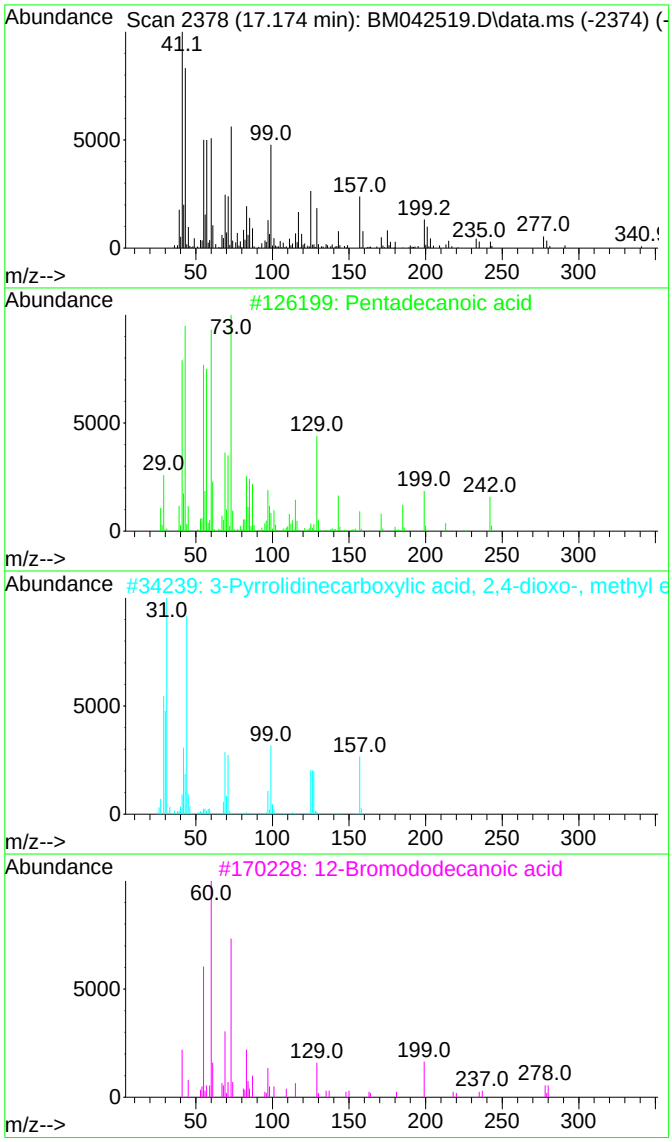
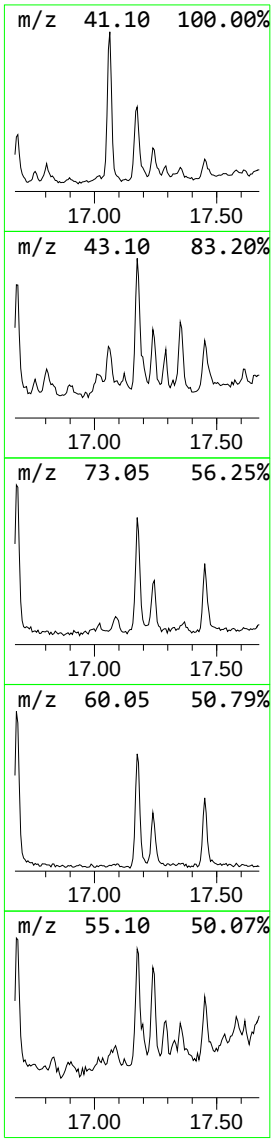
Peak Number 10 unknown17.174 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	5.54 ng	290563	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	30
2	3-Pyrrolidinecarboxylic acid, 2,...	157	C6H7NO4	051925-57-6	25
3	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	22
4	Dodecanoic acid	200	C12H24O2	000143-07-7	22
5	Tridecanoic acid	214	C13H26O2	000638-53-9	22





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Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

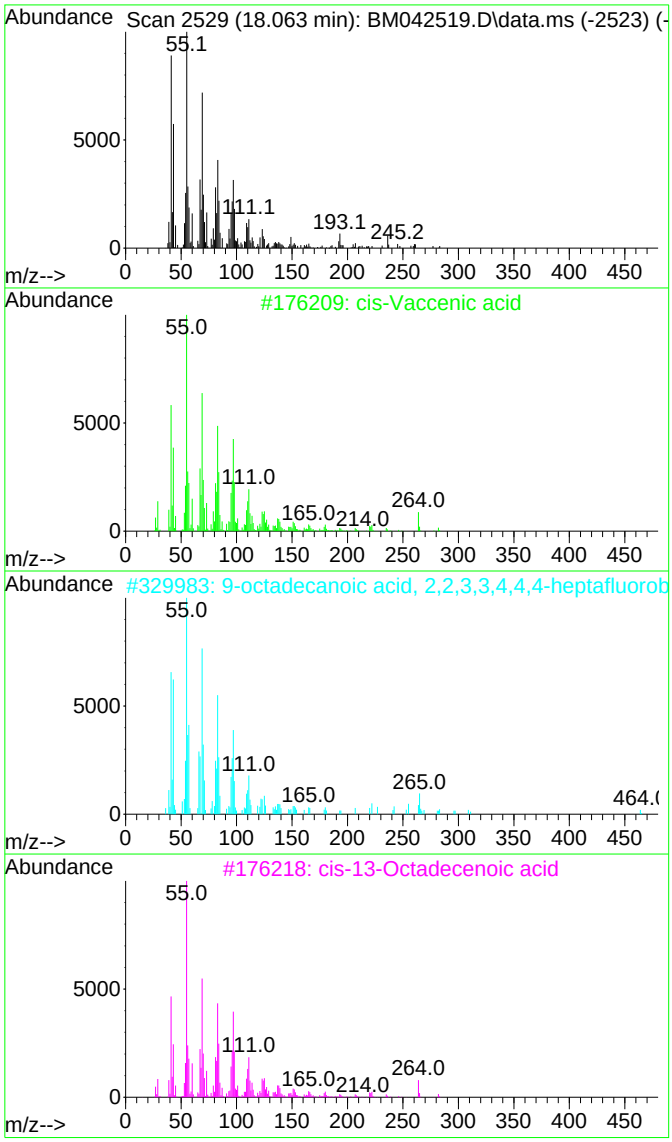
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

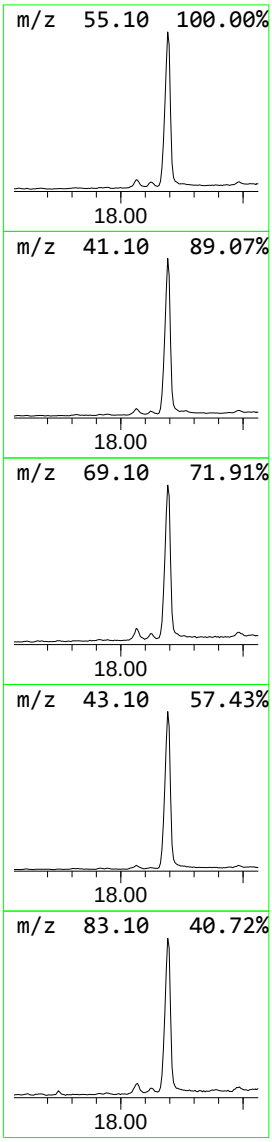
****

Peak Number 11 cis-Vaccenic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	7.08 ng	371225	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
2	9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	90
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	87
4	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	86
5	Palmitoleic acid	254	C16H30O2	000373-49-9	83





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Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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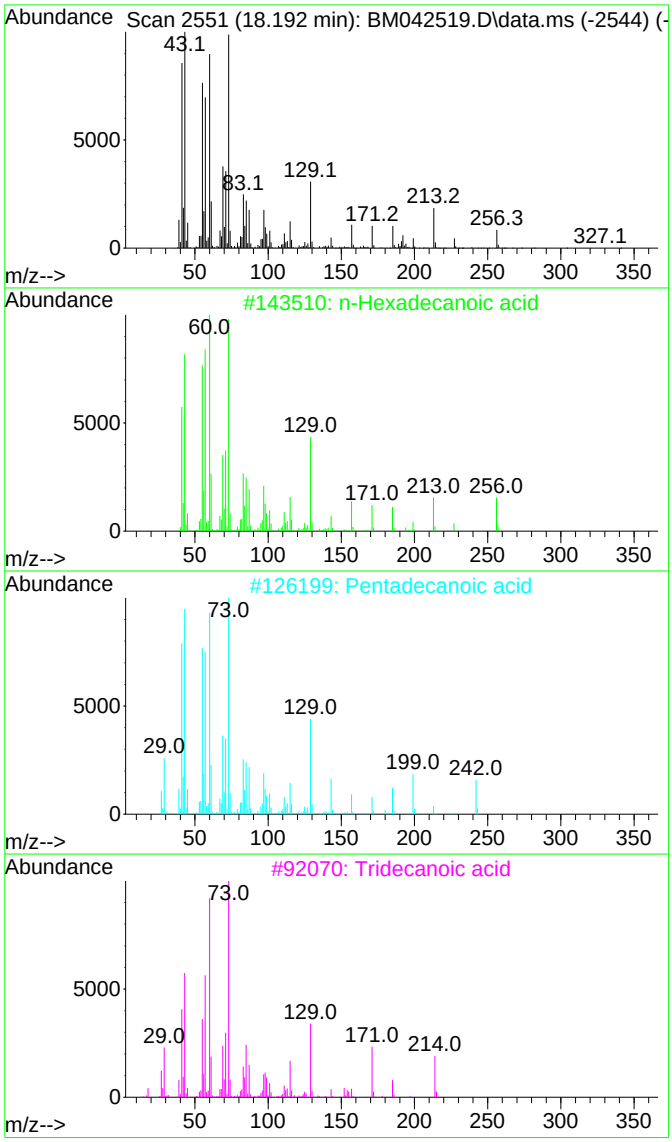
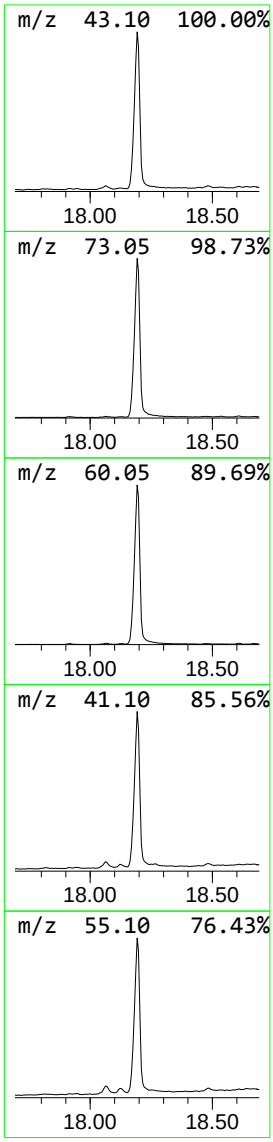
Peak Number 12 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	136.84 ng	7176710	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

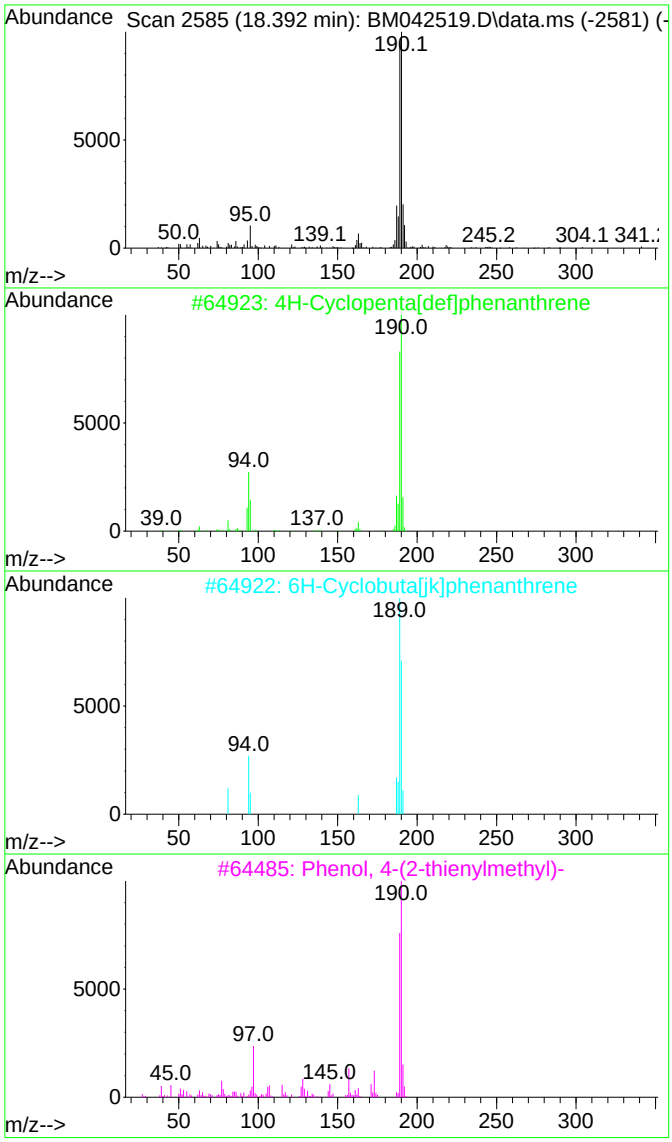
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

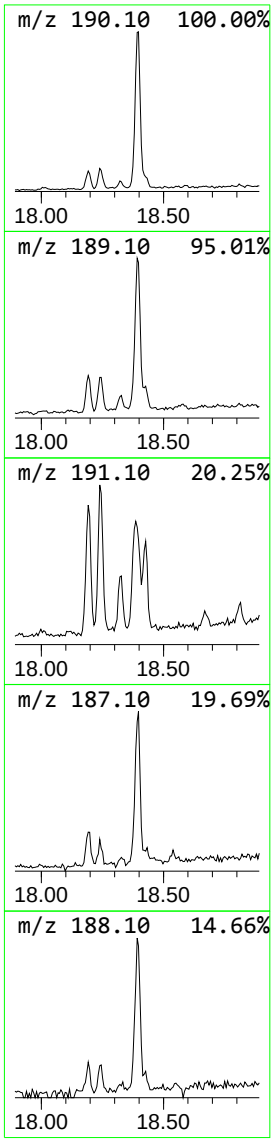
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 4H-Cyclopenta[def]phenanthrene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.392	3.62 ng	189969	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	64
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	42
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42





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Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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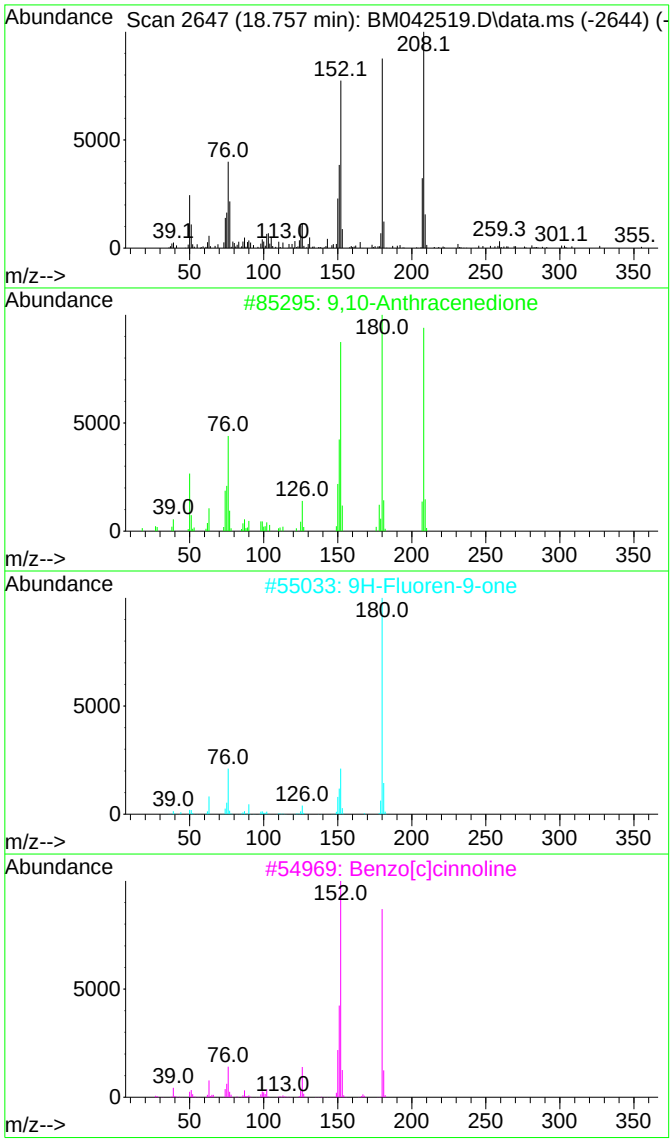
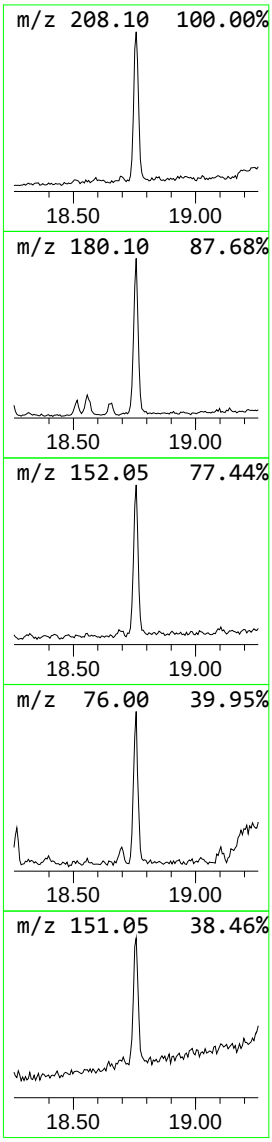
Peak Number 14 9,10-Anthracenedione Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.757	4.12 ng	216270	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	86
3	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
4	5,6-Dimethyl-1,10-phenanthroline	208	C14H12N2	003002-81-1	53
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	49





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Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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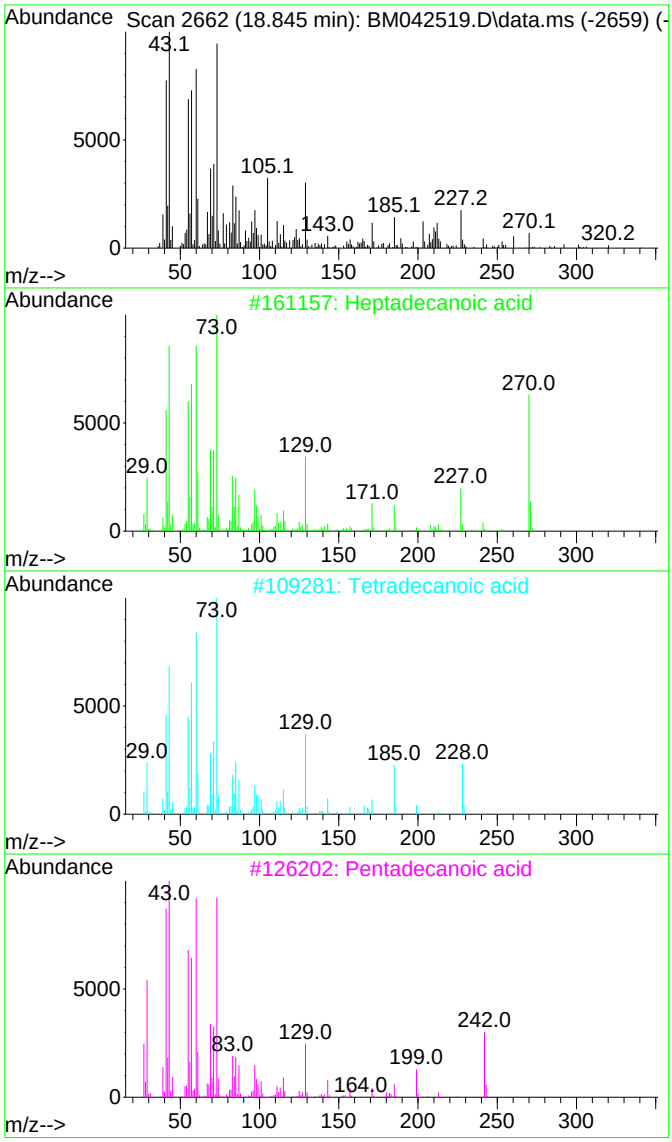
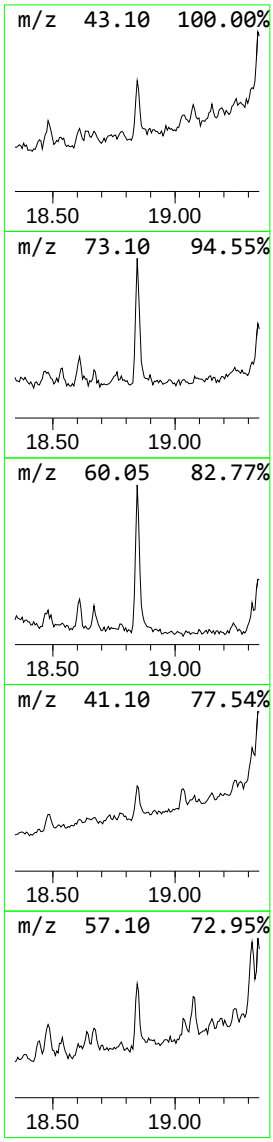
Peak Number 15 Heptadecanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.845	3.91 ng	205170	Phenanthrene-d10	17.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid	270	C17H34O2	000506-12-7	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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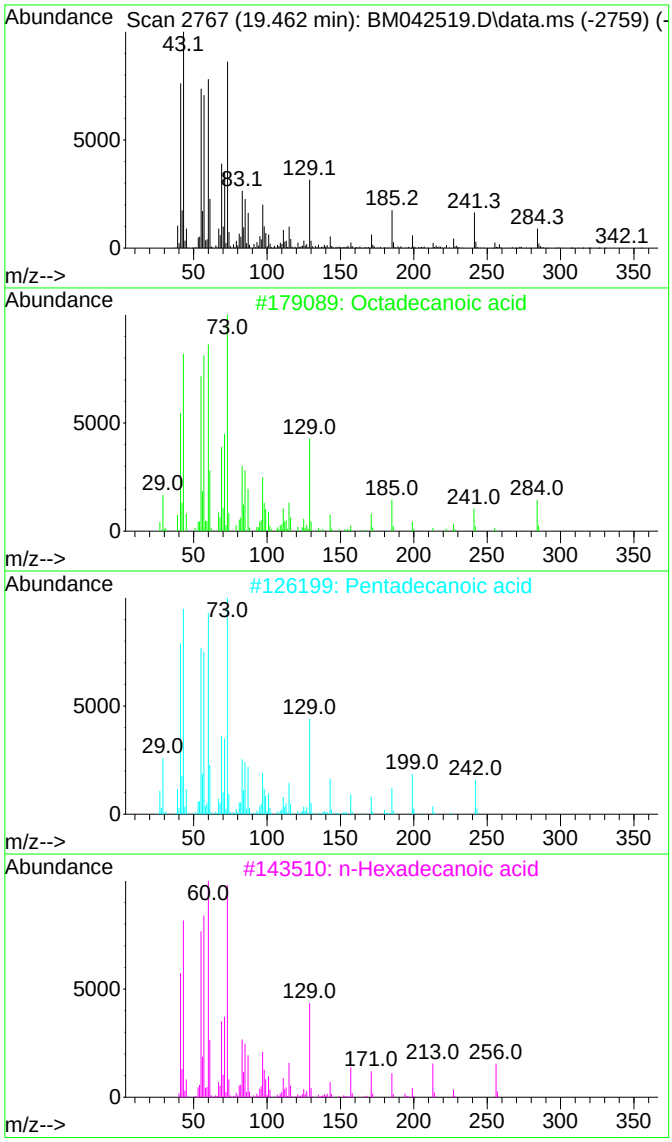
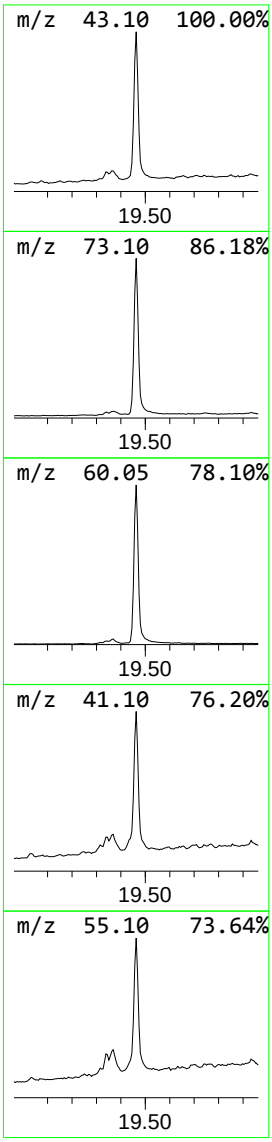
Peak Number 16 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	34.96 ng	4259030	Chrysene-d12	21.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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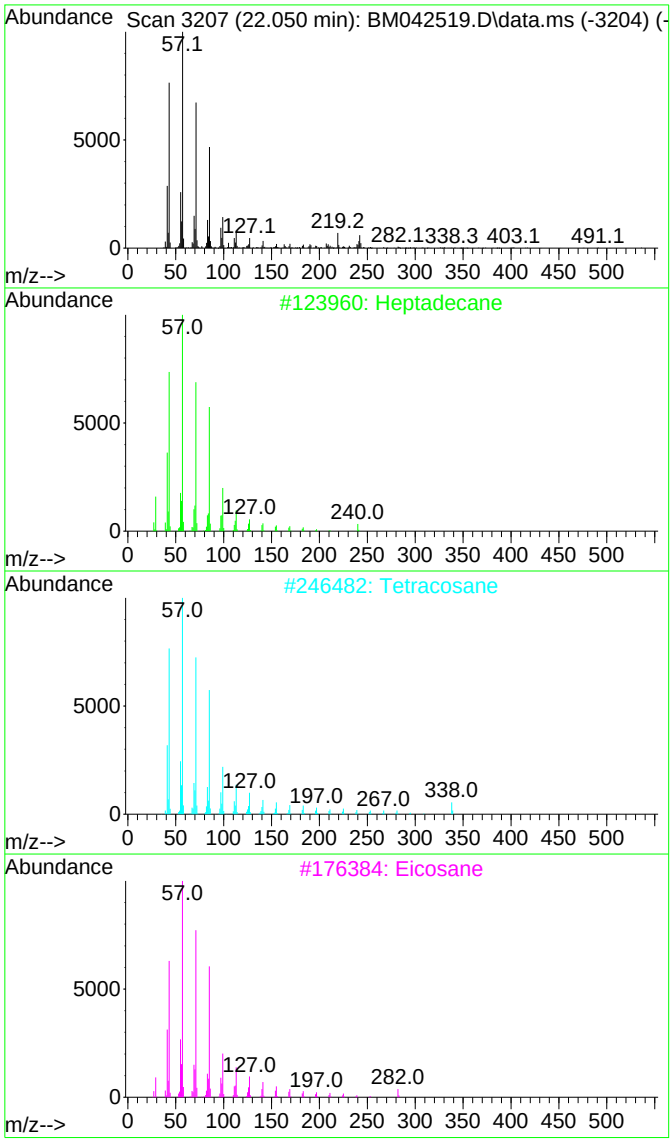
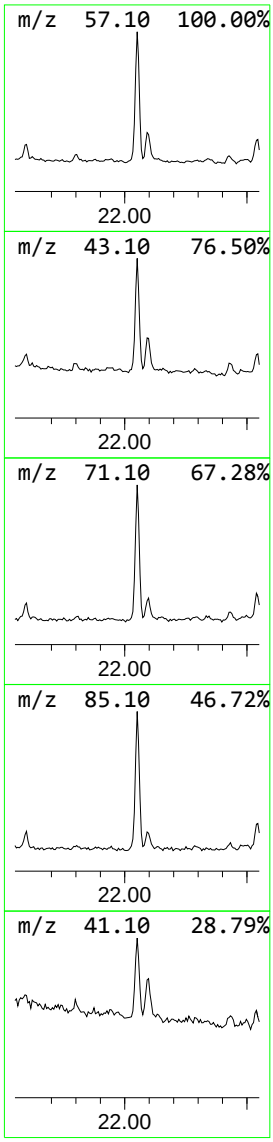
Peak Number 17 Heptadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.051	4.64 ng	565859	Chrysene-d12	21.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Tetracosane	338	C24H50	000646-31-1	94
3	Eicosane	282	C20H42	000112-95-8	93
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	86





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Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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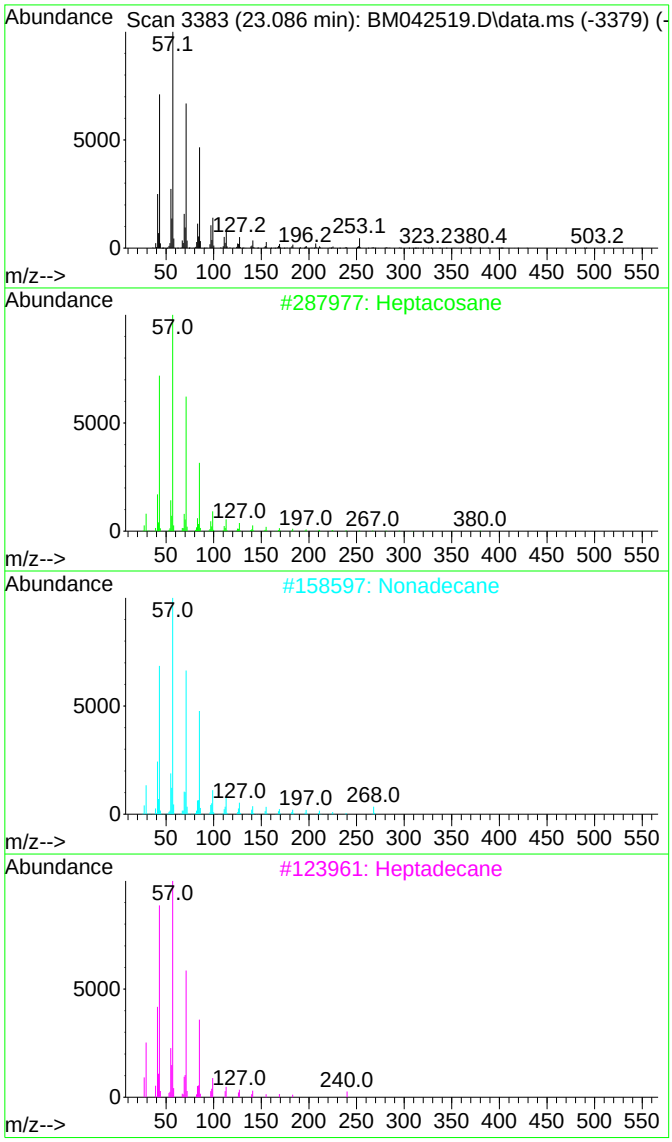
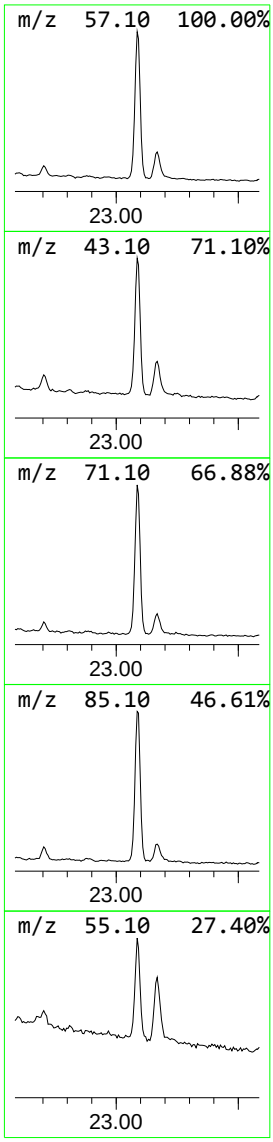
Peak Number 18 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.086	37.02 ng	1541690	Perylene-d12	23.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	95
2	Nonadecane	268	C19H40	000629-92-5	95
3	Heptadecane	240	C17H36	000629-78-7	95
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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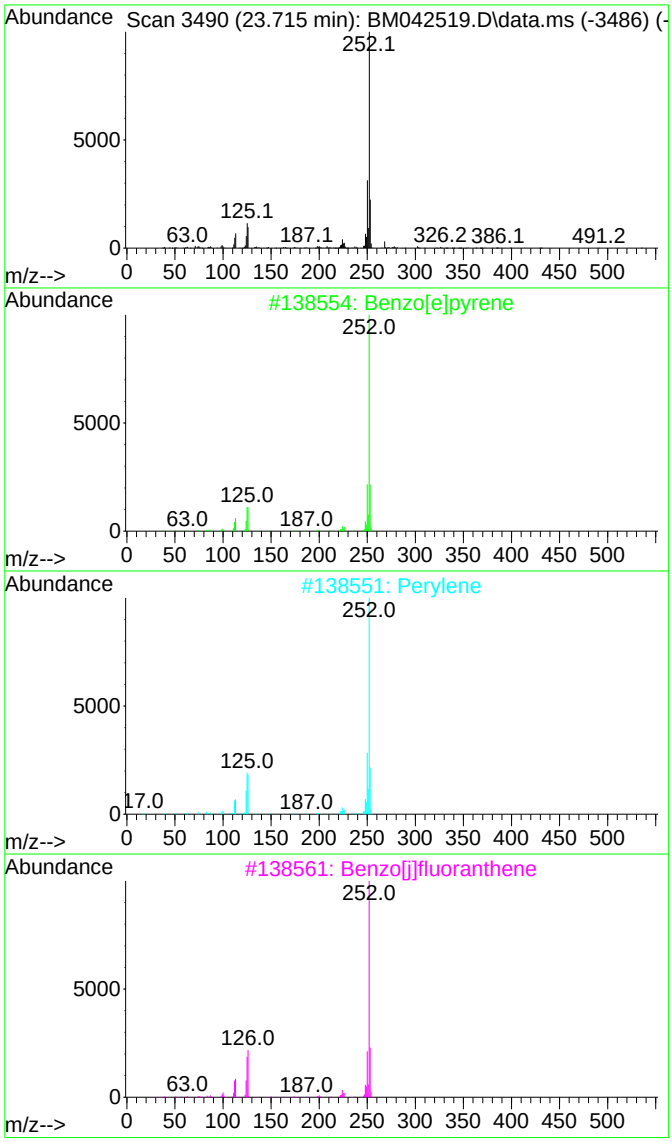
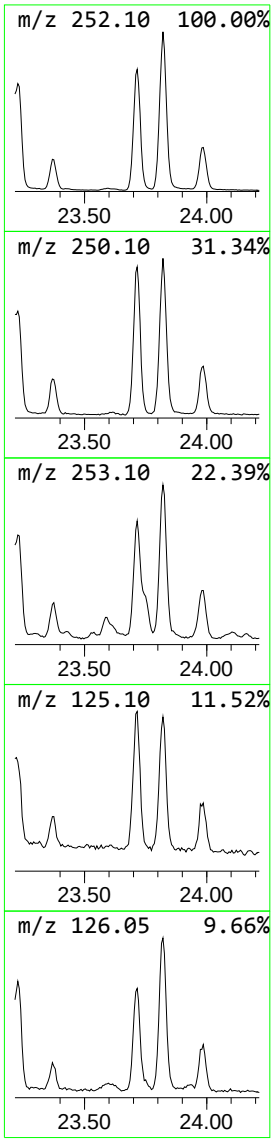
Peak Number 19 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.715	27.63 ng	1150760	Perylene-d12	23.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Perylene	252	C20H12	000198-55-0	94
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

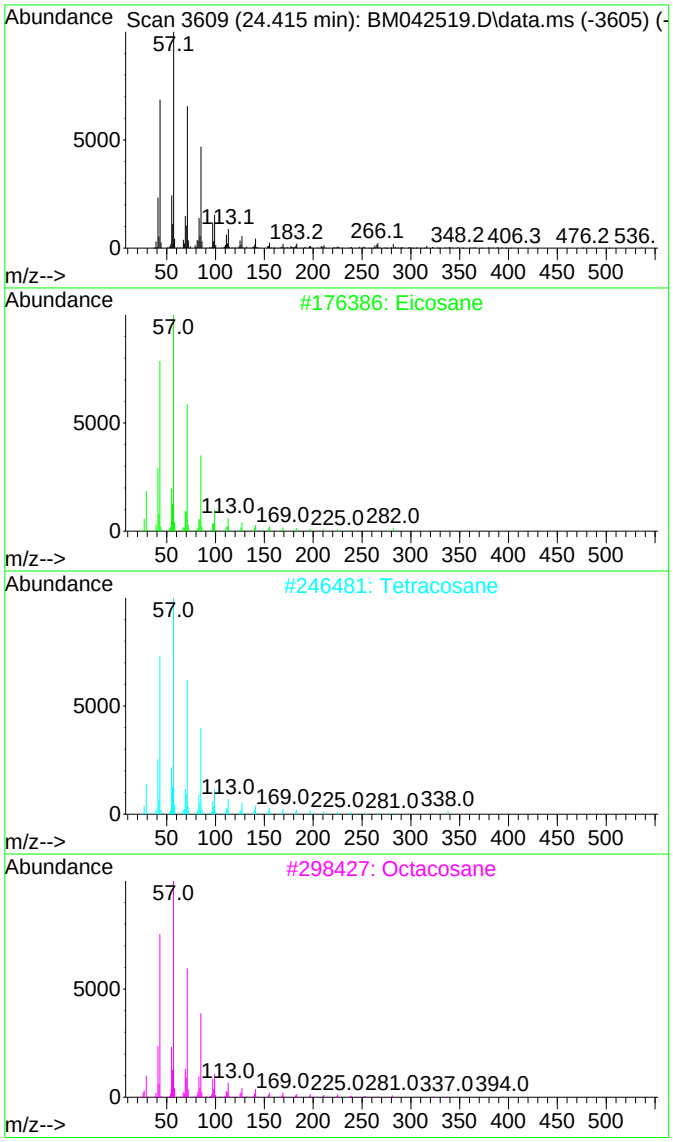
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

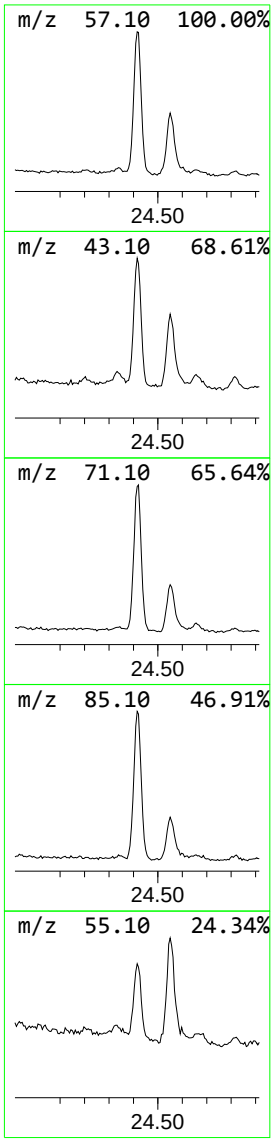
****

Peak Number 20 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.415	20.70 ng	862138	Perylene-d12	23.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Tetracosane	338	C24H50	000646-31-1	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
5	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
Data File : BM042519.D
Acq On : 31 Oct 2023 20:10
Operator : MA/JU
Sample : 04938-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
A-3(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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
Butanoic acid, ...	4.763	4.5	ng	153383	1	7.922	683602	20.0
2-Pentanone, 4-...	5.010	6.0	ng	206293	1	7.922	683602	20.0
1,3,5,7-Cyclooc...	5.875	8.7	ng	298439	1	7.922	683602	20.0
Cyclopropanecar...	12.375	4.0	ng	149852	2	10.740	744694	20.0
Phthalic anhydride	12.569	19.1	ng	712527	2	10.740	744694	20.0
1-Decene	14.186	6.2	ng	307616	3	14.569	989650	20.0
2,2,4-Trimethyl...	15.310	14.4	ng	714180	3	14.569	989650	20.0
Tetradecanoic acid	16.686	5.0	ng	262066	4	17.321	1048940	20.0
Tris(2-chloropr...	17.063	6.3	ng	327788	4	17.321	1048940	20.0
unknown17.174	17.174	5.5	ng	290563	4	17.321	1048940	20.0
cis-Vaccenic acid	18.063	7.1	ng	371225	4	17.321	1048940	20.0
n-Hexadecanoic ...	18.192	136.8	ng	7176710	4	17.321	1048940	20.0
4H-Cyclopenta[d...	18.392	3.6	ng	189969	4	17.321	1048940	20.0
9,10-Anthracene...	18.757	4.1	ng	216270	4	17.321	1048940	20.0
Heptadecanoic acid	18.845	3.9	ng	205170	4	17.321	1048940	20.0
Octadecanoic acid	19.462	35.0	ng	4259030	5	21.509	2436630	20.0
Heptadecane	22.051	4.6	ng	565859	5	21.509	2436630	20.0
Heptacosane	23.086	37.0	ng	1541690	6	23.933	832894	20.0
Benzo[e]pyrene	23.715	27.6	ng	1150760	6	23.933	832894	20.0
Eicosane	24.415	20.7	ng	862138	6	23.933	832894	20.0