LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

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-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047416.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.263	60	64	73	rBV	113960	175312	2.32%	0.256%
2	4.557	277	284	295	rVB	158883	233858	3.09%	0.341%
3	5.010	354	361	380	rBV	2568394	3924955	51.92%	5.721%
4	6.569	619	626	647	rBV	2292254	3885198	51.40%	5.663%
5	7.340	750	757	769	rBV	826589	1317757	17.43%	1.921%
6	8.492	946	953	971	rBV	1467804	2565169	33.93%	3.739%
7	10.098	1218	1226	1241	rBV	954944	1670082	22.09%	2.434%
8	10.875	1352	1358	1368	rBV	54154	130787	1.73%	0.191%
9	12.610	1645	1653	1675	rBV	3816222	5934957	78.51%	8.651%
10	13.727	1838	1843	1857	rVB	98196	173805	2.30%	0.253%
11	14.004	1883	1890	1898	rBV	1403995	2116316	28.00%	3.085%
12	14.069	1898	1901	1908	rVB	56808	91944	1.22%	0.134%
13	15.392	2118	2126	2134	rBV	181837	301183	3.98%	0.439%
14	15.521	2140	2148	2167	rBV	2722963	4271986	56.51%	6.227%
15	15.763	2184	2189	2199	rVB5	44713	80234	1.06%	0.117%
16	16.592	2327	2330	2341	rVB	46621	81771	1.08%	0.119%
17	16.774	2355	2361	2365	rBV	1663836	2408901	31.87%	3.511%
18	16.815	2365	2368	2377	rVV	948809	1257166	16.63%	1.833%
19	16.910	2379	2384	2389	rVV	219012	320923	4.25%	0.468%
20	17.198	2425	2433	2444	rBV3	77719	205639	2.72%	0.300%
21	17.651	2506	2510	2515	rBV	141458	215742	2.85%	0.314%
22	17.704	2515	2519	2528	rBV	705416	1074717	14.22%	1.567%
23	17.845	2538	2543	2547	rBV3	239847	411955	5.45%	0.600%
24	17.886	2547	2550	2558	rVB	101519	162018	2.14%	0.236%
25	18.162	2593	2597	2602	rBV	91036	111550	1.48%	0.163%
26	18.215	2602	2606	2611	rBV	138950	192746	2.55%	0.281%
27	18.586	2665	2669	2674	rBV	115084	195503	2.59%	0.285%
28	18.645	2675	2679	2683	rVV3	64628	113271	1.50%	0.165%
29	18.739	2690	2695	2701	rBV2	99395	174542	2.31%	0.254%
30	18.851	2709	2714	2722	rBV	2368760	3230588	42.74%	4.709%
31	19.009	2737	2741	2748	rBV	310794	482495	6.38%	0.703%
32	19.221	2768	2777	2787	rBV	2154284	3399651	44.97%	4.956%
33	19.304	2787	2791	2797	rVB2	87850	147464	1.95%	0.215%
34	19.439	2806	2814	2819	rBV	6255829	7559113	100.00%	11.019%
35	19.562	2829	2835	2841	rBV4	128428	306036	4.05%	0.446%
36	19.692	2853	2857	2859	rBV3	139847	210837	2.79%	0.307%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

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-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.733	2861	2864	2869	rVB	282625	373887	4.95%	0.545%
38	19.833	2877	2881	2884	rBV	203667	243285	3.22%	0.355%
39	19.886	2886	2890	2894	rVV2	186367	278644	3.69%	0.406%
40	20.027	2911	2914	2918	rBV	135787	148357	1.96%	0.216%
41	20.074	2919	2922	2926	rBV	110512	160023	2.12%	0.233%
42	20.233	2947	2949	2953	rBV	95037	85204	1.13%	0.124%
43	20.745	3030	3036	3042	rBV3	533061	956766	12.66%	1.395%
44	20.950	3067	3071	3075	rBV	1120811	1360502	18.00%	1.983%
45	21.015	3075	3082	3086	rVV2	2316915	4674152	61.83%	6.813%
46	21.056	3086	3089	3102	rVB	1130343	1745846	23.10%	2.545%
47	21.186	3108	3111	3114	rVB	183928	201471	2.67%	0.294%
48	22.039	3252	3256	3264	rVB	740008	1140175	15.08%	1.662%
49	22.880	3393	3399	3404	rBV	995458	2358451	31.20%	3.438%
50	23.468	3494	3499	3511	rVB	570086	1331117	17.61%	1.940%
51	23.591	3514	3520	3531	rVB	834401	1821976	24.10%	2.656%
52	23.715	3535	3541	3548	rBV	1185124	2586906	34.22%	3.771%

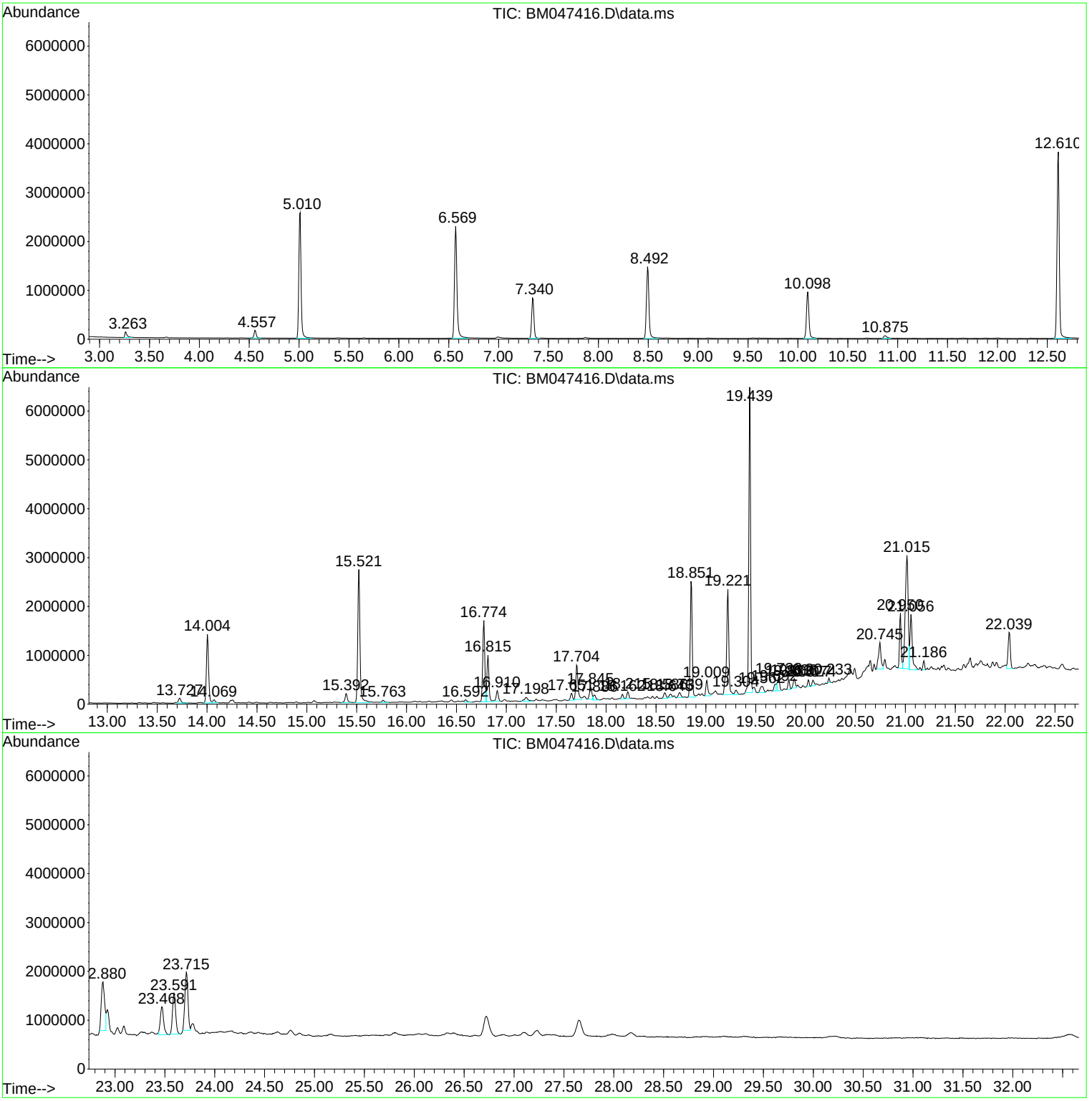
Sum of corrected areas: 68602933

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

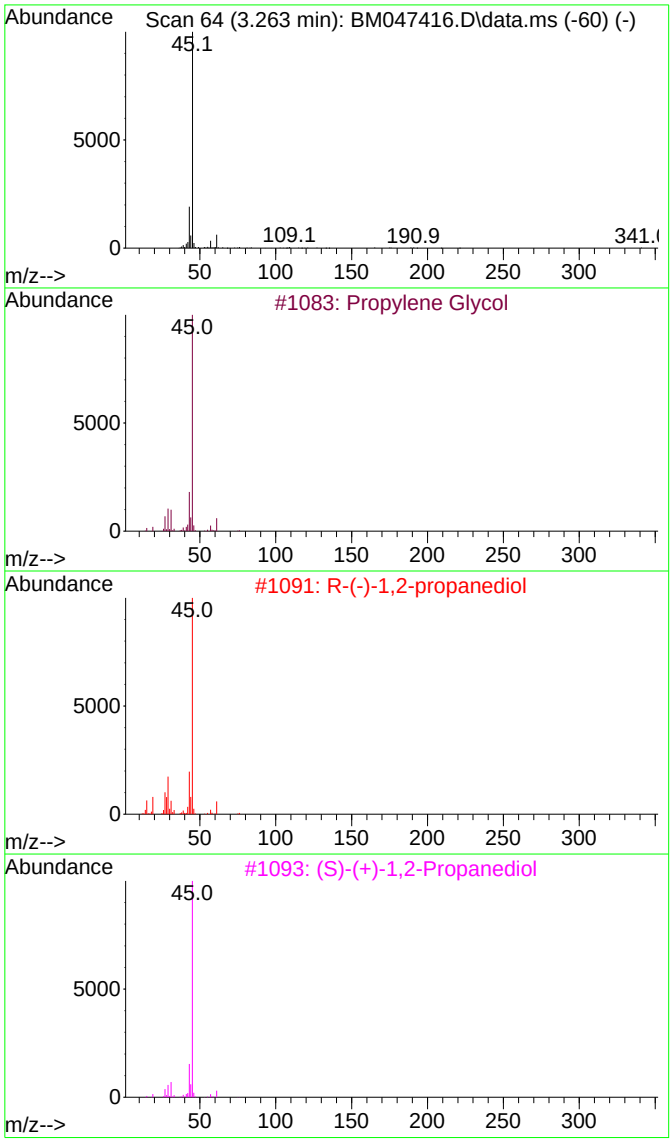
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

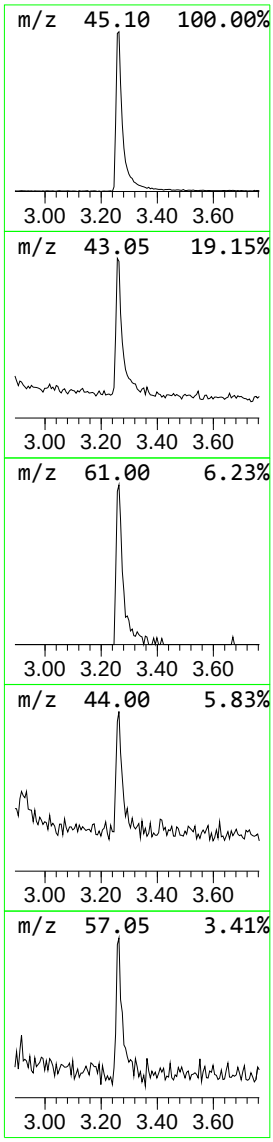
****

Peak Number 1 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.263	2.66 ng	175312	1,4-Dichlorobenzene-d4	7.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4	2-Butanol	74	C4H10O	000078-92-2	40
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

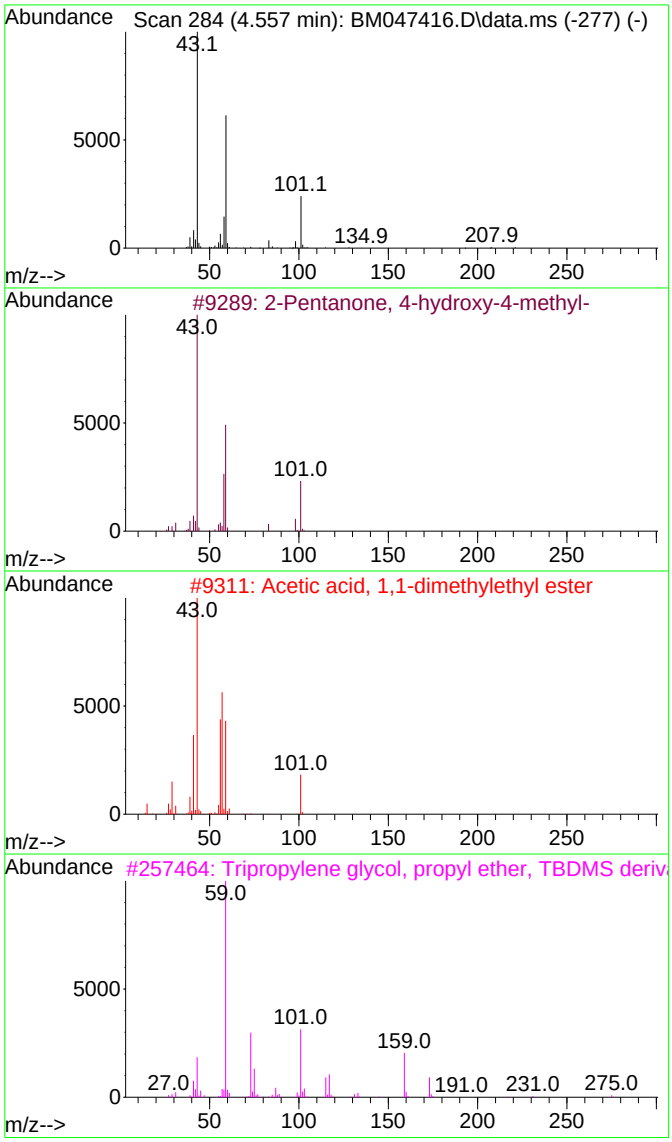
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

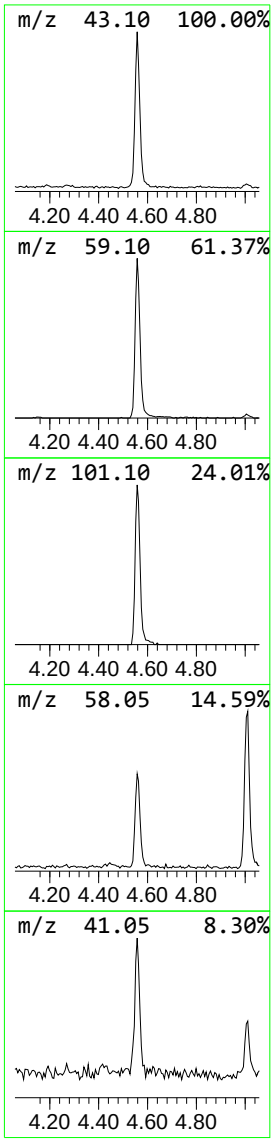
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	3.55 ng	233858	1,4-Dichlorobenzene-d4	7.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Tripropylene glycol, propyl ethe...	348	C18H40O4Si	1000367-07-2	28
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

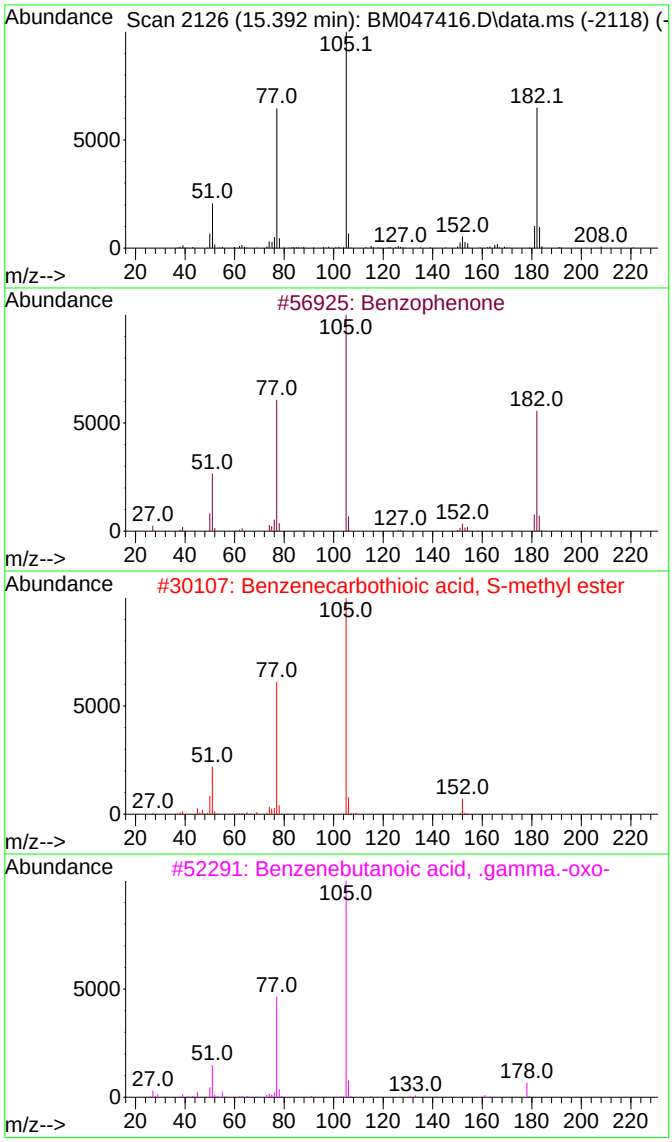
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

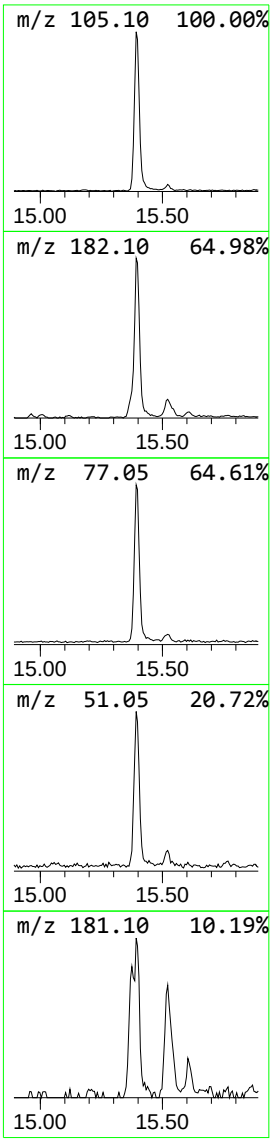
****

Peak Number 3 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	2.50 ng	301183	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43
4	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	43
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

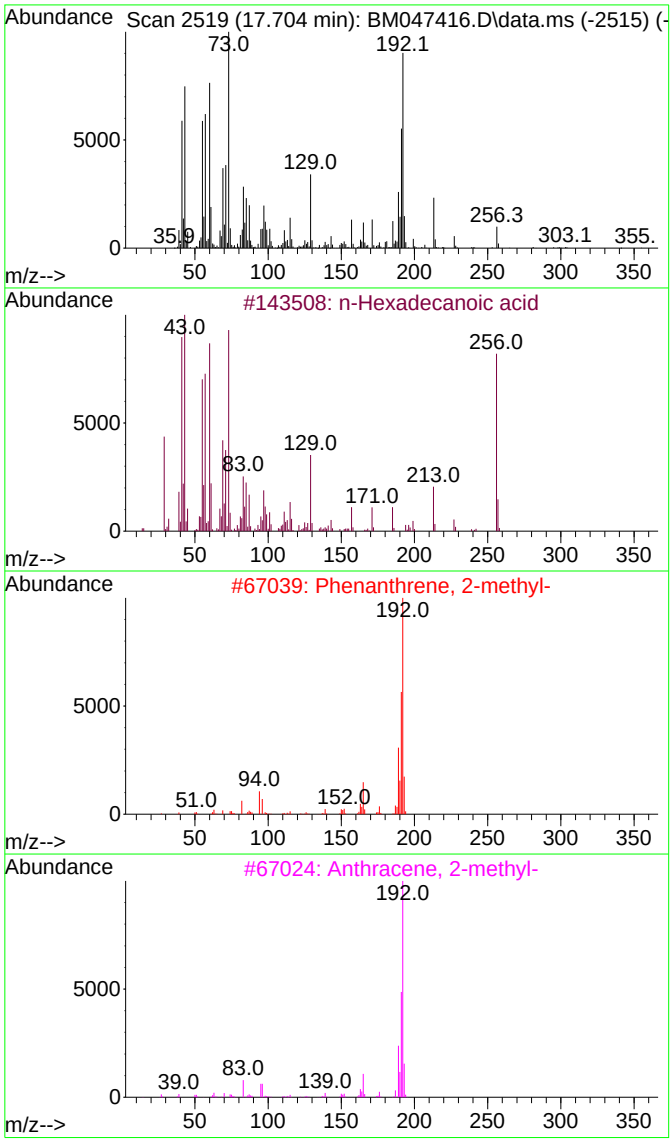
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

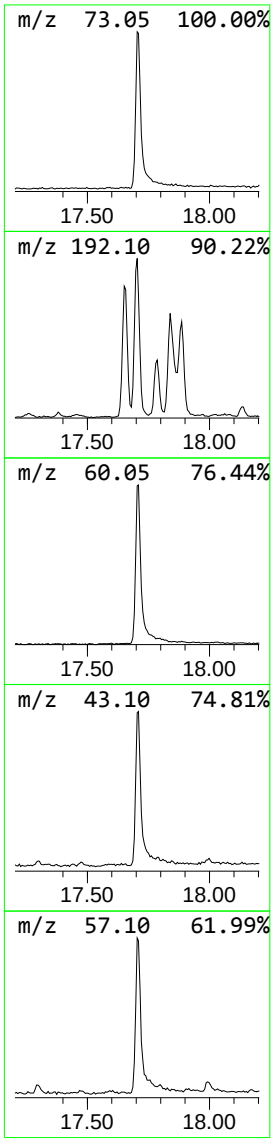
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.704	8.92 ng	1074720	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
5	Tridecanoic acid	214	C13H26O2	000638-53-9	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

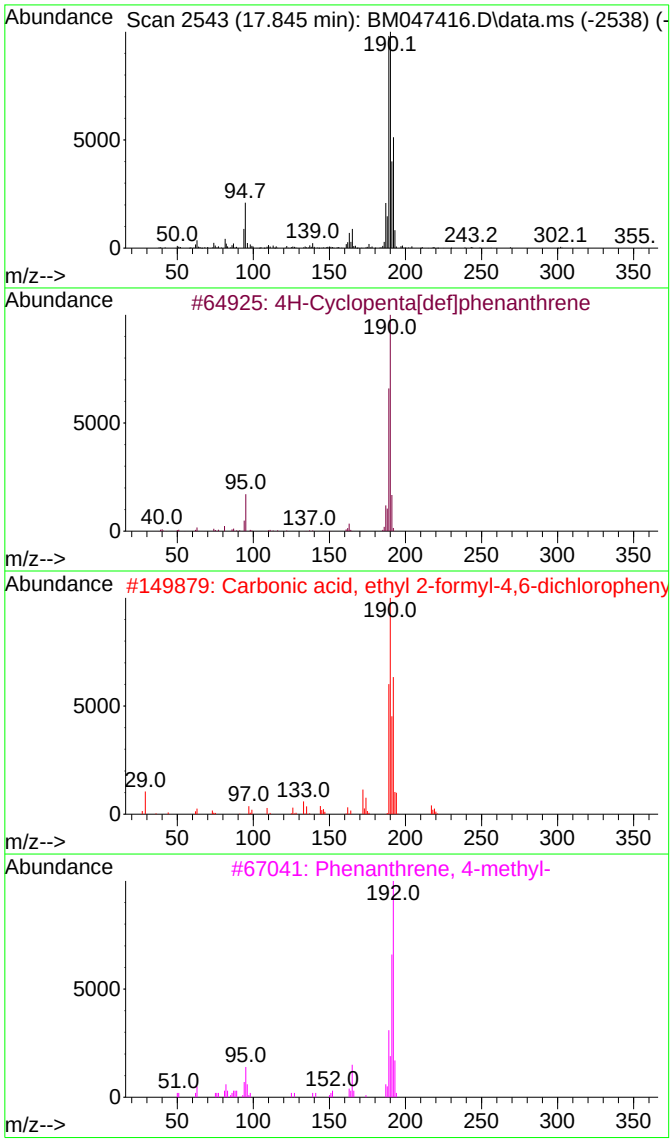
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

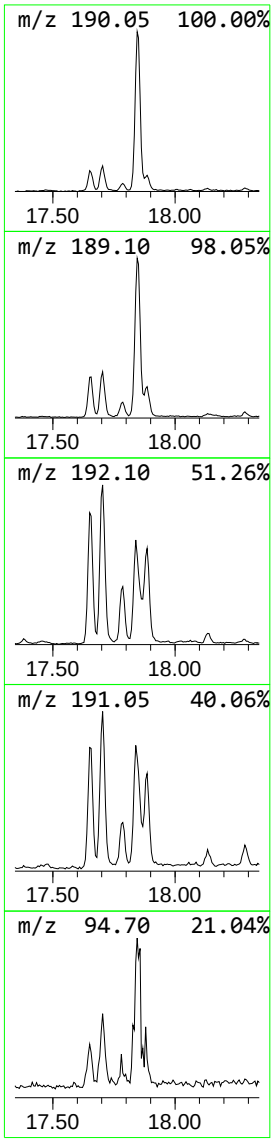
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.845	3.42 ng	411955	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	22
4	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	22
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

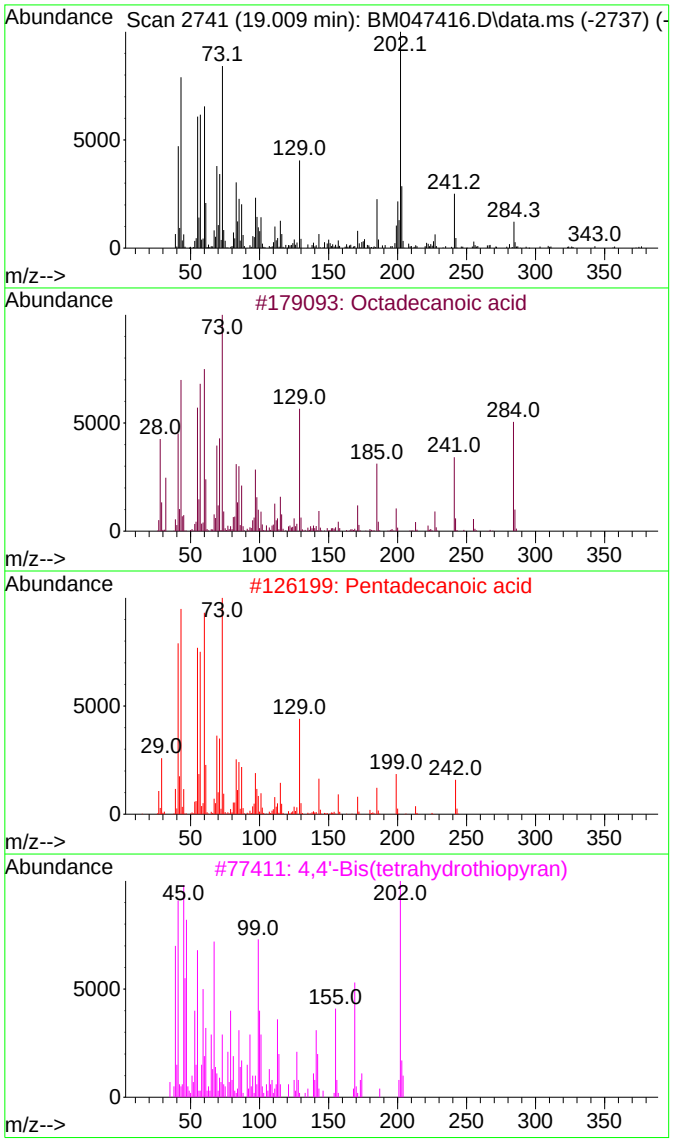
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

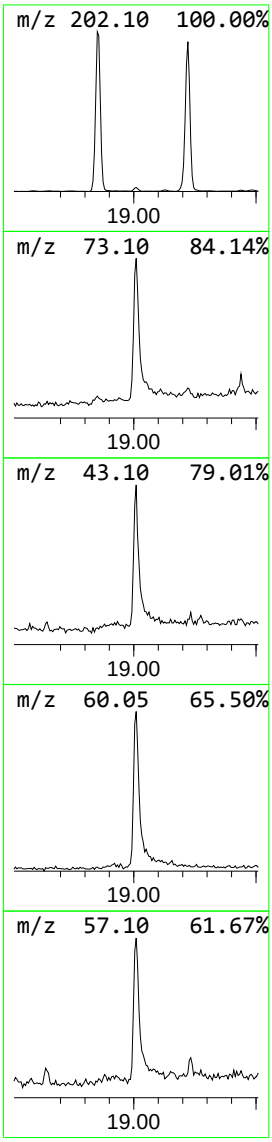
****

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	2.06 ng	482495	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	56
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	45
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

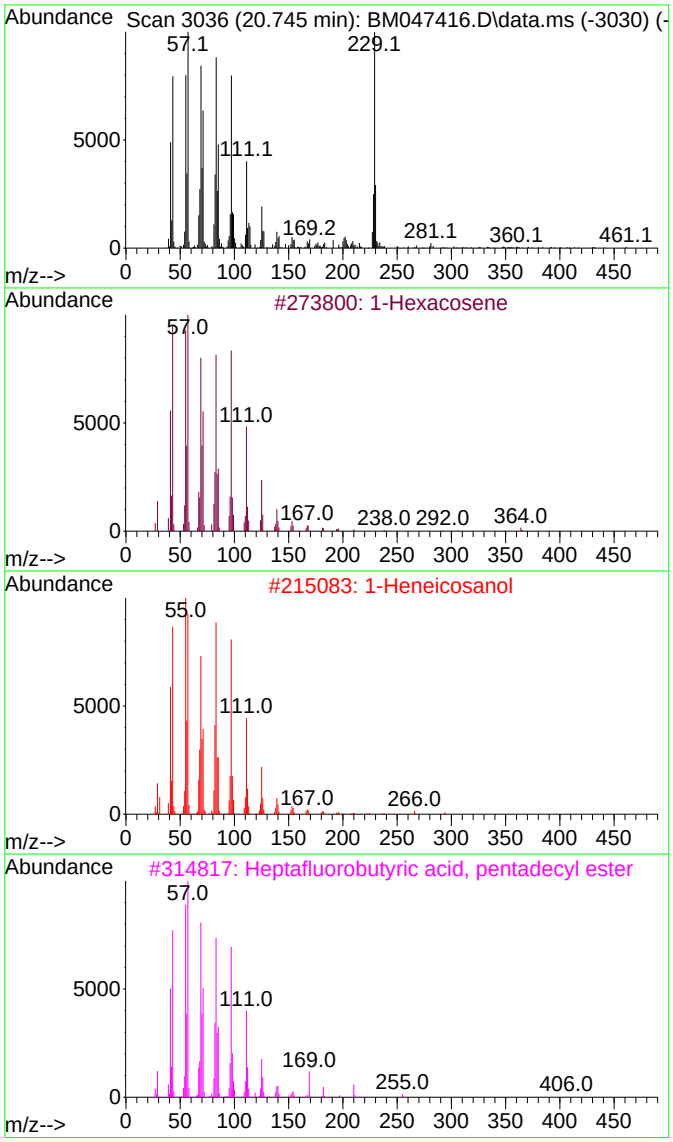
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

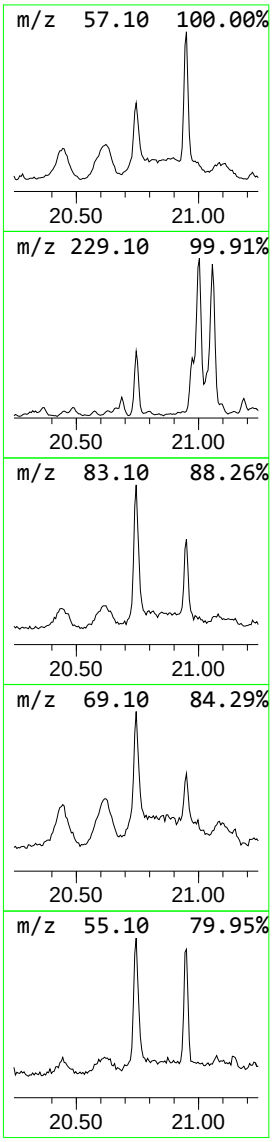
****

Peak Number 7 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.745	4.09 ng	956766	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	83
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	78
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

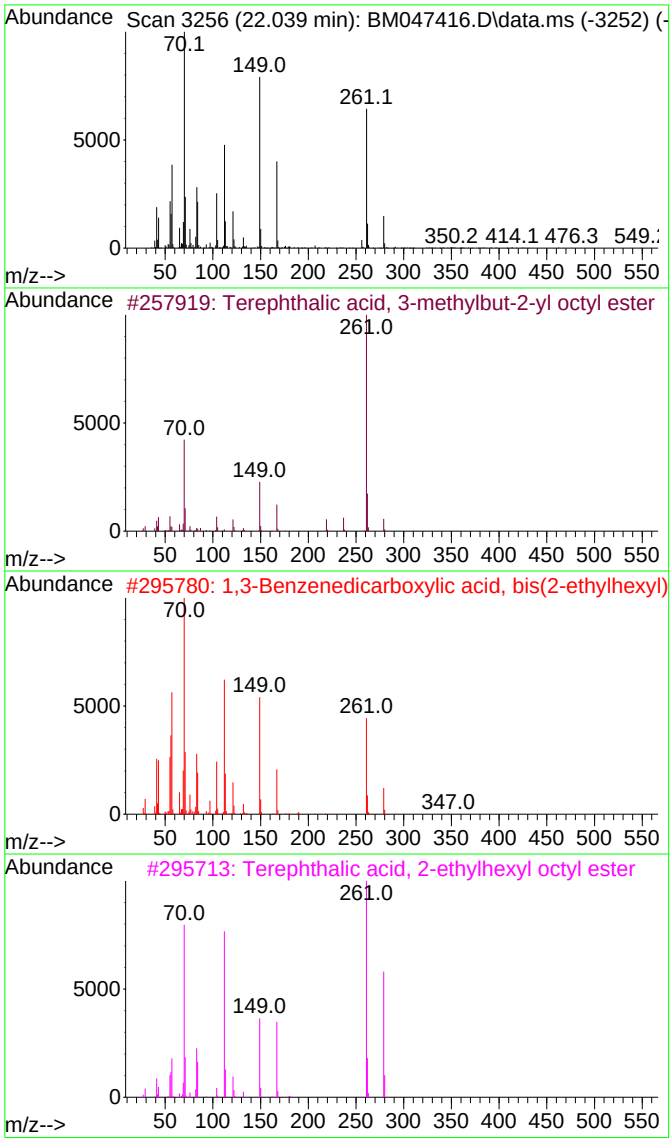
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

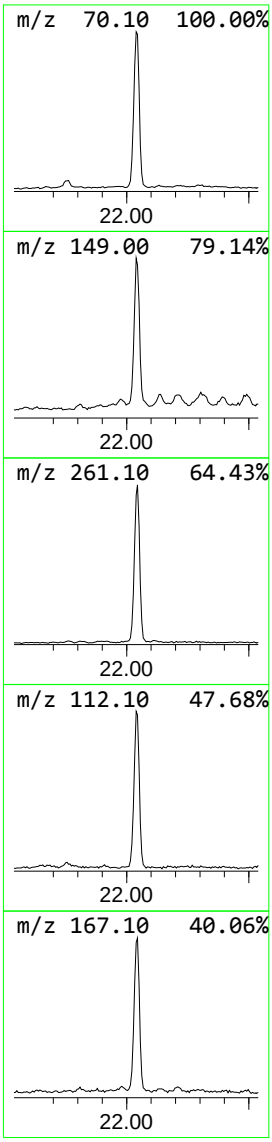
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Terephthalic acid, 3-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.039	4.88 ng	1140180	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
4	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	47
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

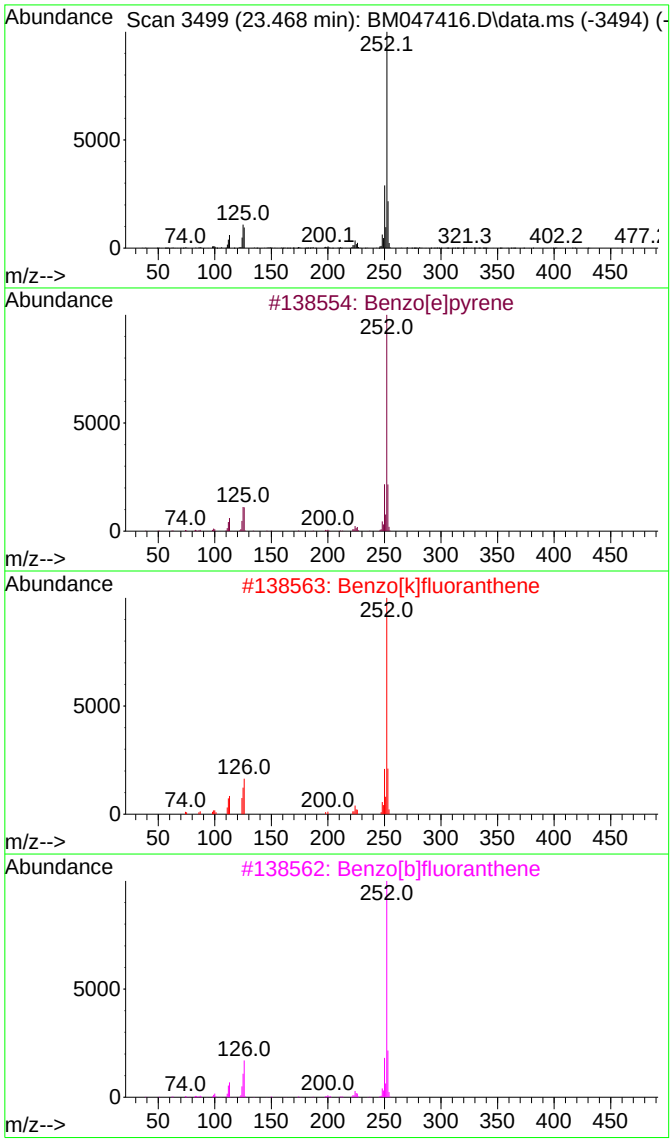
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

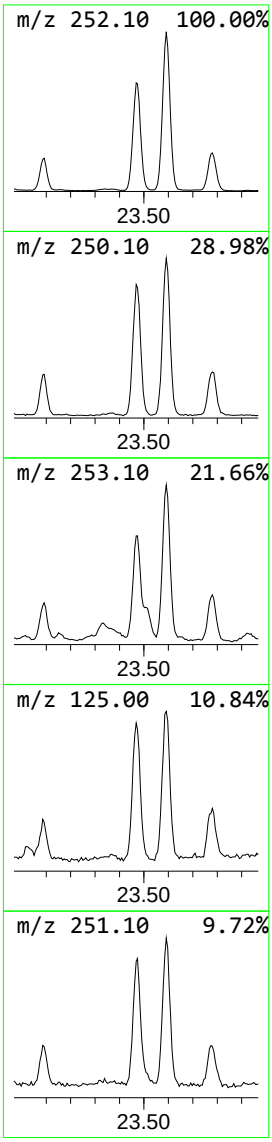
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.468	10.29 ng	1331120	Perylene-d12	23.715

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Perylene	252	C20H12	000198-55-0	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047416.D
Acq On : 30 Aug 2024 21:38
Operator : RC/JU
Sample : P3793-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT2864

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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
Propylene Glycol	3.263	2.7	ng	175312	1	7.345	1317760	20.0
2-Pentanone, 4-...	4.557	3.5	ng	233858	1	7.345	1317760	20.0
Benzophenone	15.392	2.5	ng	301183	4	16.774	2408900	20.0
n-Hexadecanoic ...	17.704	8.9	ng	1074720	4	16.774	2408900	20.0
4H-Cyclopenta[d...	17.845	3.4	ng	411955	4	16.774	2408900	20.0
Octadecanoic acid	19.009	2.1	ng	482495	5	21.015	4674150	20.0
1-Hexacosene	20.745	4.1	ng	956766	5	21.015	4674150	20.0
Terephthalic ac...	22.039	4.9	ng	1140180	5	21.015	4674150	20.0
Benzo[e]pyrene	23.468	10.3	ng	1331120	6	23.715	2586910	20.0