LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

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_P\Methods\8270E-BP072723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP016448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.587	385	391	401	rVB	981275	1397886	7.70%	1.392%
2	6.387	519	527	539	rBV	109764	210839	1.16%	0.210%
3	7.028	623	636	646	rBV3	143858	440208	2.43%	0.438%
4	7.211	659	667	678	rVB	625596	1000172	5.51%	0.996%
5	7.658	736	743	749	rBV	271423	408681	2.25%	0.407%
6	7.811	764	769	778	rVB2	194055	300967	1.66%	0.300%
7	8.081	806	815	827	rBV	1899729	3099464	17.08%	3.086%
8	9.275	1009	1018	1026	rBV	3241700	5373566	29.61%	5.350%
9	10.910	1289	1296	1304	rBV	2718368	4519510	24.90%	4.500%
10	13.351	1698	1711	1718	rBV	8643351	12702833	69.99%	12.647%
11	13.587	1743	1751	1761	rBV	6301495	10089682	55.59%	10.045%
12	14.181	1842	1852	1861	rBV	109414	193381	1.07%	0.193%
13	14.728	1936	1945	1957	rVB	4217572	6082484	33.51%	6.056%
14	14.928	1970	1979	1988	rBV	899637	1252632	6.90%	1.247%
15	16.092	2170	2177	2184	rBV	158375	235905	1.30%	0.235%
16	16.222	2190	2199	2207	rBV	2664099	3860468	21.27%	3.843%
17	16.534	2247	2252	2256	rBV	134429	188449	1.04%	0.188%
18	16.728	2280	2285	2295	rBV	154514	230150	1.27%	0.229%
19	16.840	2299	2304	2310	rBV2	126468	218570	1.20%	0.218%
20	17.492	2409	2415	2422	rBV	4964028	7198487	39.66%	7.167%
21	18.122	2518	2522	2530	rVB	156641	197525	1.09%	0.197%
22	18.345	2554	2560	2571	rBV	2134241	3171763	17.48%	3.158%
23	18.428	2571	2574	2586	rVB	122277	258561	1.42%	0.257%
24	19.128	2689	2693	2697	rVB	171180	217630	1.20%	0.217%
25	19.228	2706	2710	2712	rBV2	156274	207655	1.14%	0.207%
26	19.257	2712	2715	2728	rVB	758473	895716	4.94%	0.892%
27	19.381	2729	2736	2741	rVV2	116997	191427	1.05%	0.191%
28	19.475	2747	2752	2758	rVB	598148	672120	3.70%	0.669%
29	19.569	2764	2768	2782	rBV2	714547	1138333	6.27%	1.133%
30	20.039	2843	2848	2854	rBV	14221158	18150116	100.00%	18.070%
31	20.639	2947	2950	2956	rVB	186593	223325	1.23%	0.222%
32	20.792	2972	2976	2979	rBV	181769	186829	1.03%	0.186%
33	21.257	3050	3055	3060	rBV	2059864	2746149	15.13%	2.734%
34	21.592	3106	3112	3120	rVB	4996398	6417092	35.36%	6.389%
35	23.422	3418	3423	3431	rVB3	613417	1065611	5.87%	1.061%
36	24.192	3546	3554	3569	rVB	2694093	5697466	31.39%	5.672%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

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_P\Methods\8270E-BP072723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

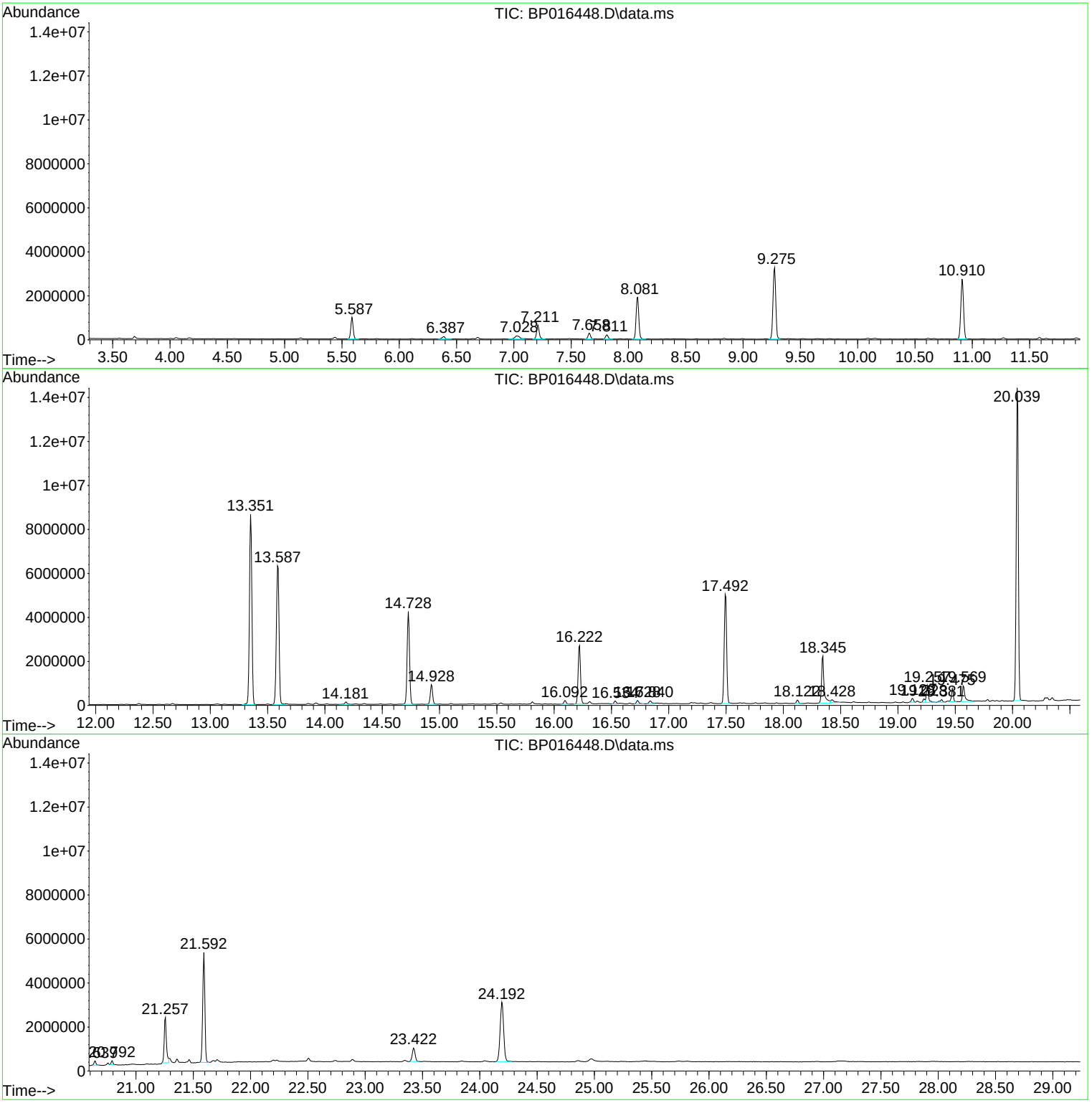
Sum of corrected areas: 100441652

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

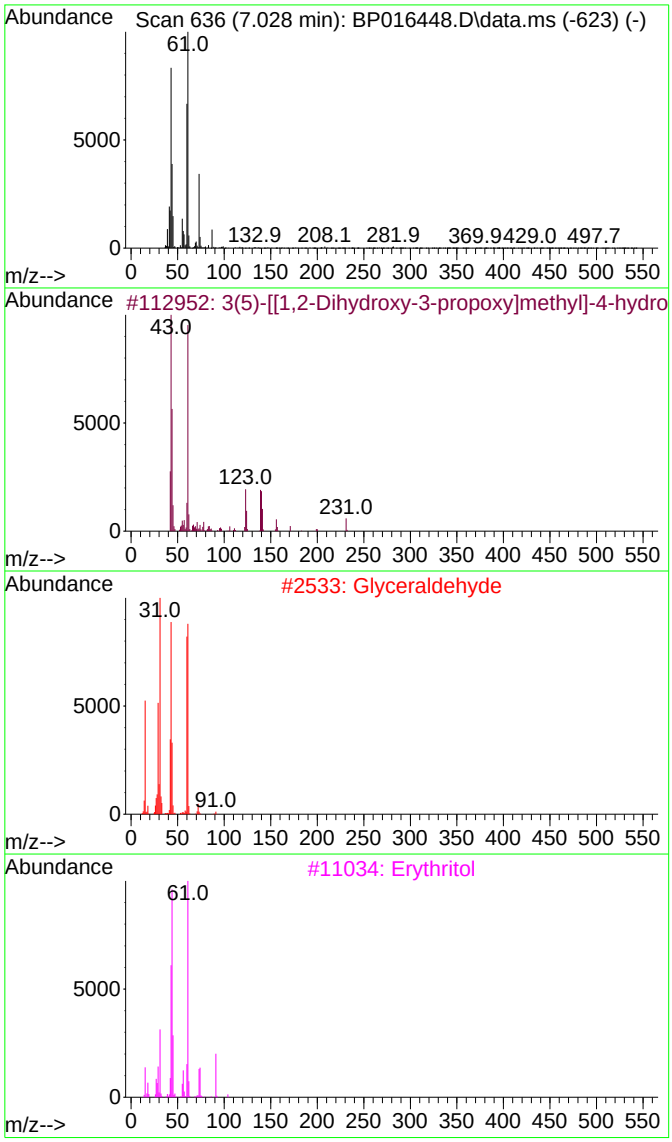
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

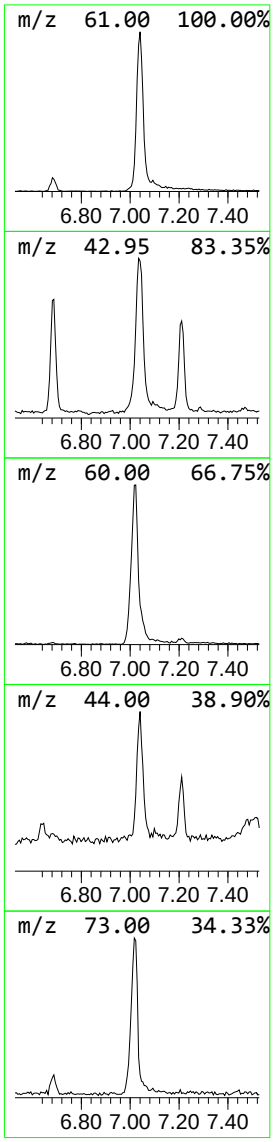
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3(5)-[[1,2-Dihydroxy-3-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.028	2.84 ng	440208	1,4-Dichlorobenzene-d4	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(5)-[[1,2-Dihydroxy-3-propoxy]m...	231	C8H13N3O5	1000211-65-4	59
2	Glyceraldehyde	90	C3H6O3	000056-82-6	50
3	Erythritol	122	C4H10O4	000149-32-6	50
4	Glycerin	92	C3H8O3	000056-81-5	42
5	2-Acetamido-d-mannitol	239	C8H17NO7	1000124-70-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

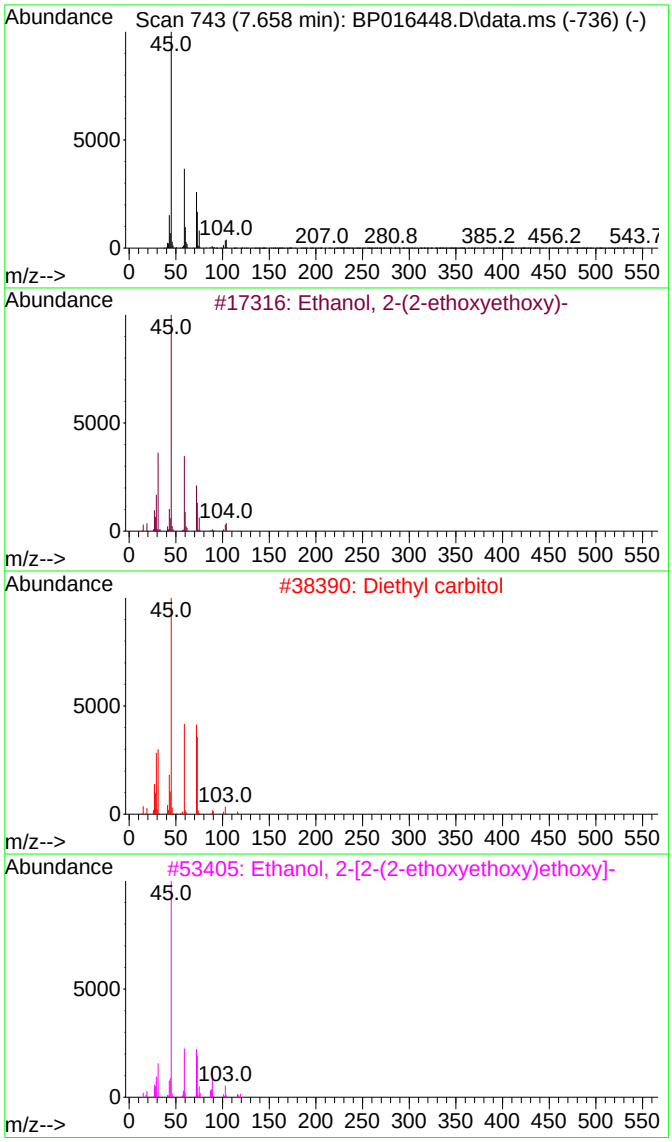
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

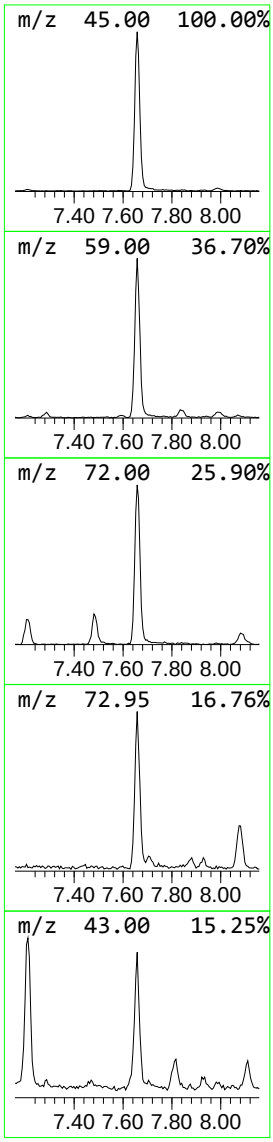
****

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.658	2.64 ng	408681	1,4-Dichlorobenzene-d4	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

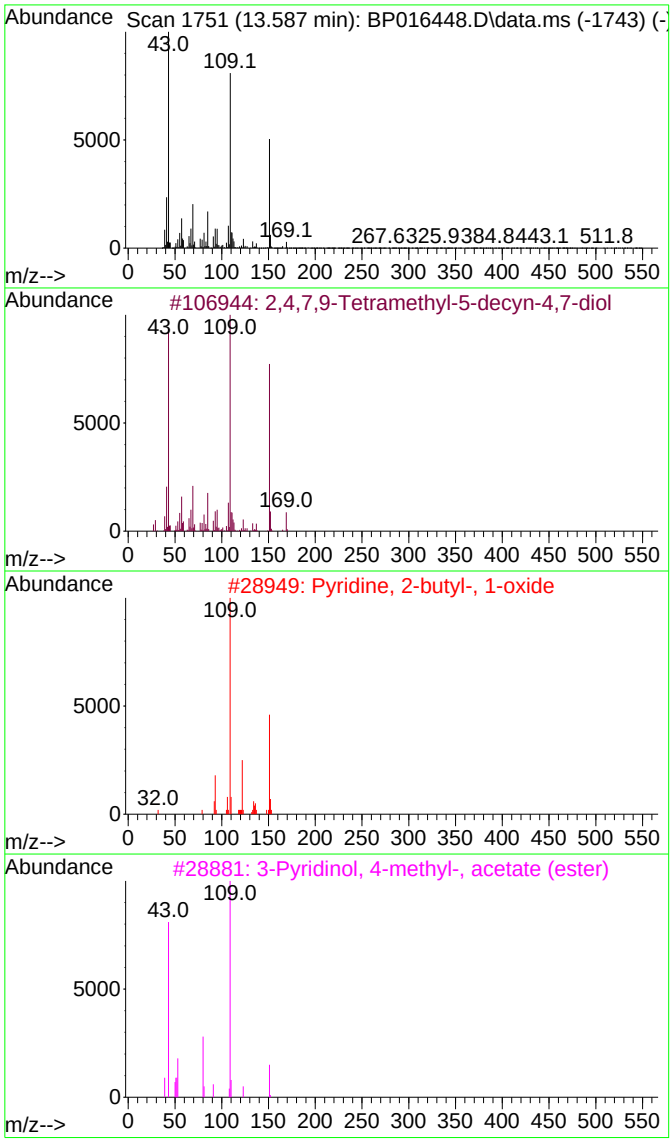
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

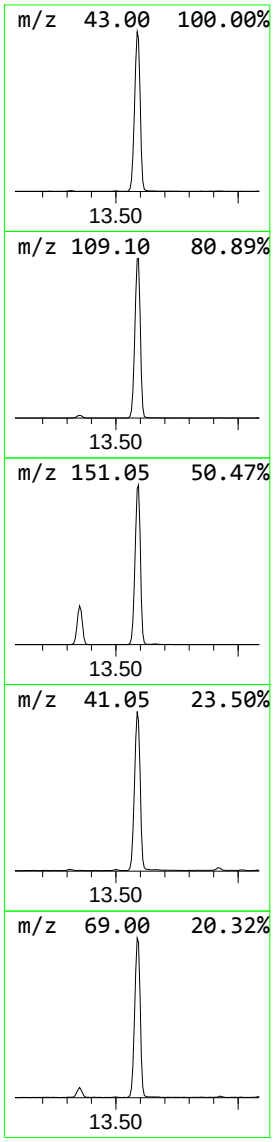
****

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	33.18 ng	10089700	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
5	Metacetamol	151	C8H9NO2	000621-42-1	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

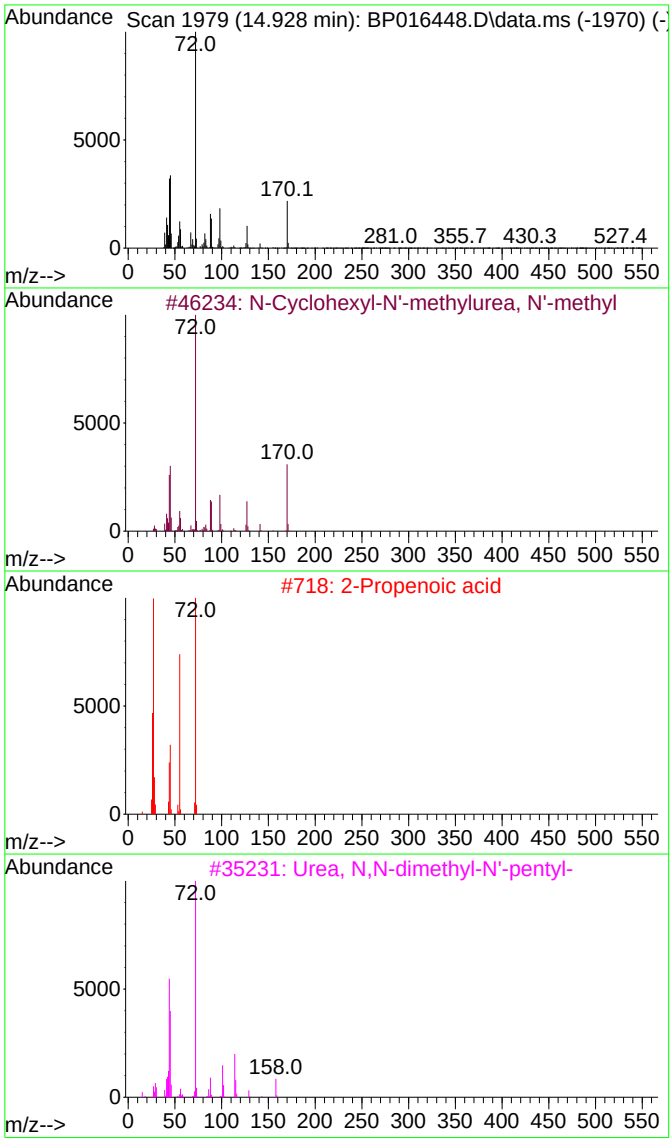
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

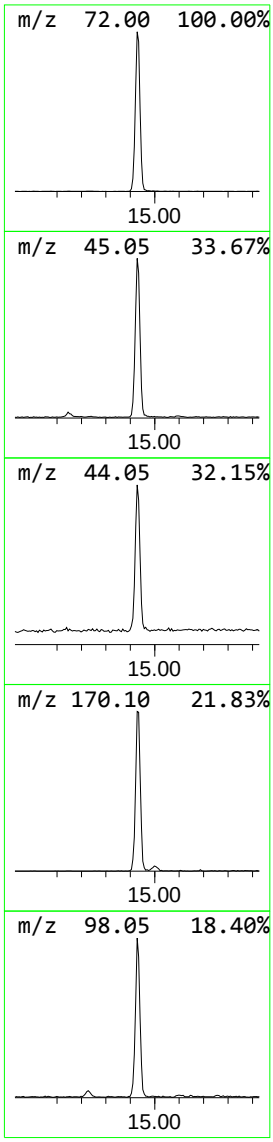
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 N-Cyclohexyl-N'-methylurea,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.928	4.12 ng	1252630	Acenaphthene-d10	14.728

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Cyclohexyl-N'-methylurea, N'-m...	170	C9H18N2O	031468-12-9	96
2	2-Propenoic acid	72	C3H4O2	000079-10-7	50
3	Urea, N,N-dimethyl-N'-pentyl-	158	C8H18N2O	1000419-88-1	40
4	Propanediamide, 2,2-diethyl-N,N,...	214	C11H22N2O2	042948-58-3	38
5	D-(-)-Norvaline	117	C5H11NO2	002013-12-9	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
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Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

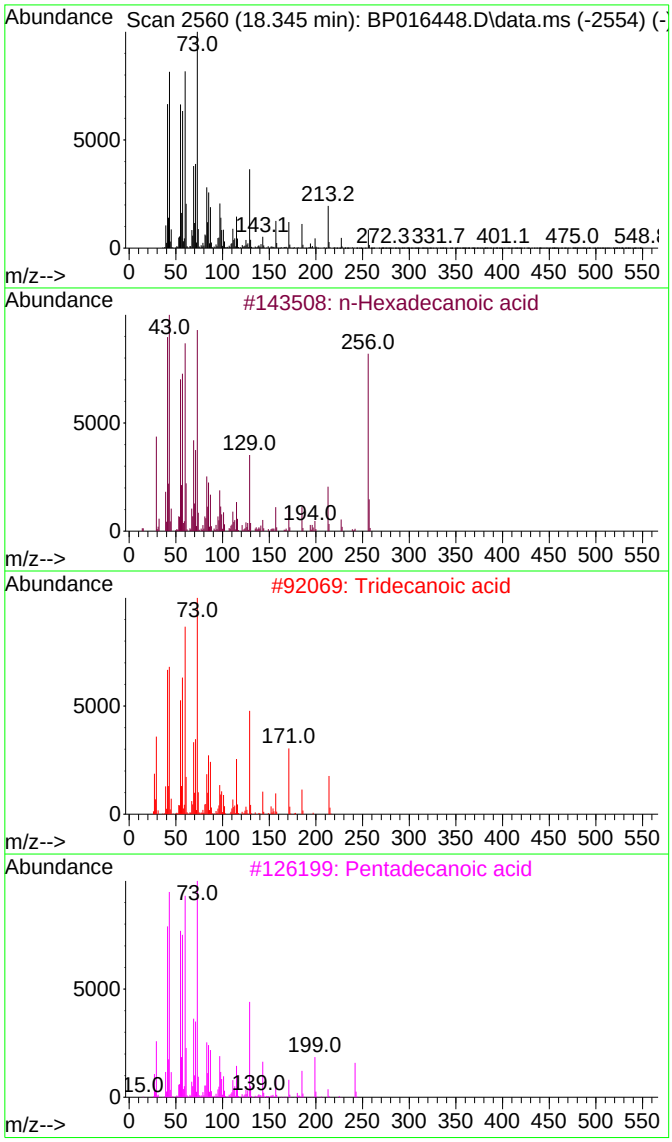
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

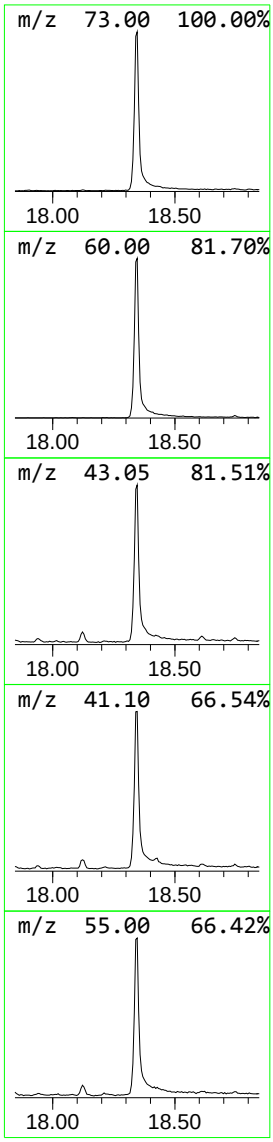
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	8.81 ng	3171760	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55





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Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
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MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

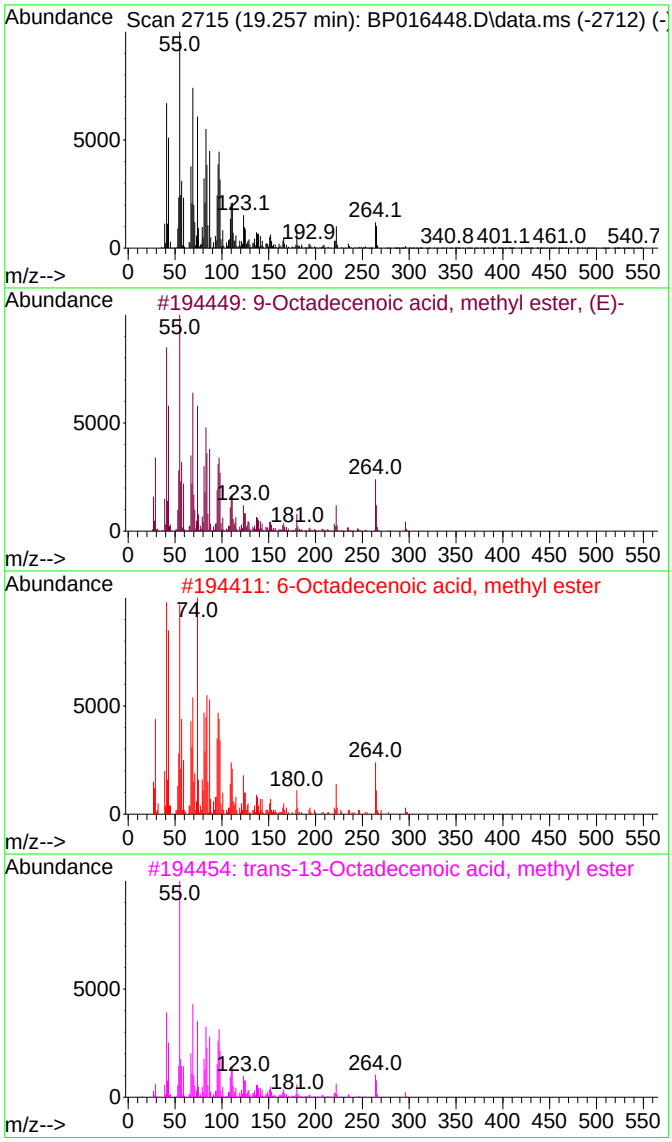
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

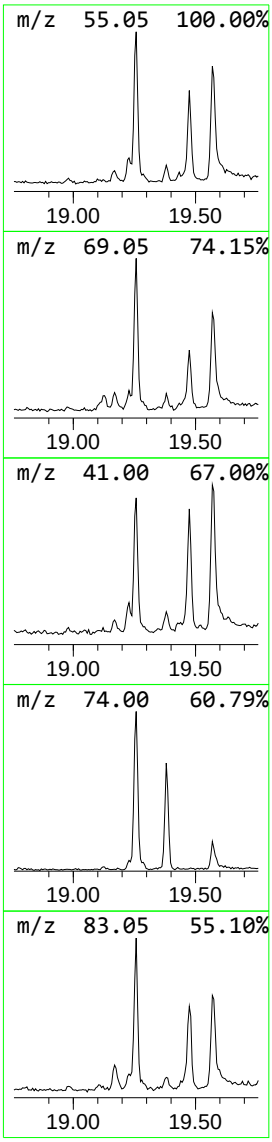
****

Peak Number 6 9-Octadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.257	2.49 ng	895716	Phenanthrene-d10	17.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
4	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

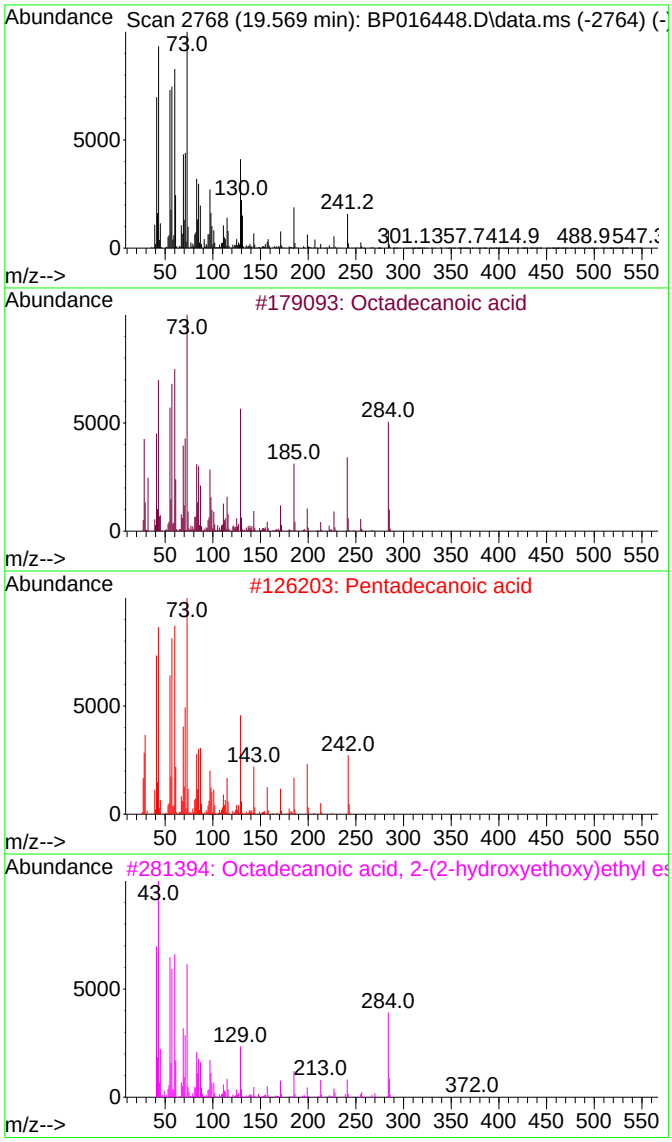
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

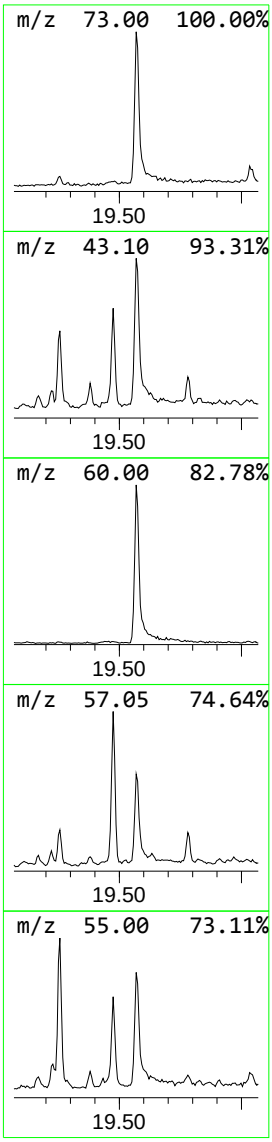
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.569	3.55 ng	1138330	Chrysene-d12	21.592

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	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





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Data File : BP016448.D
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Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

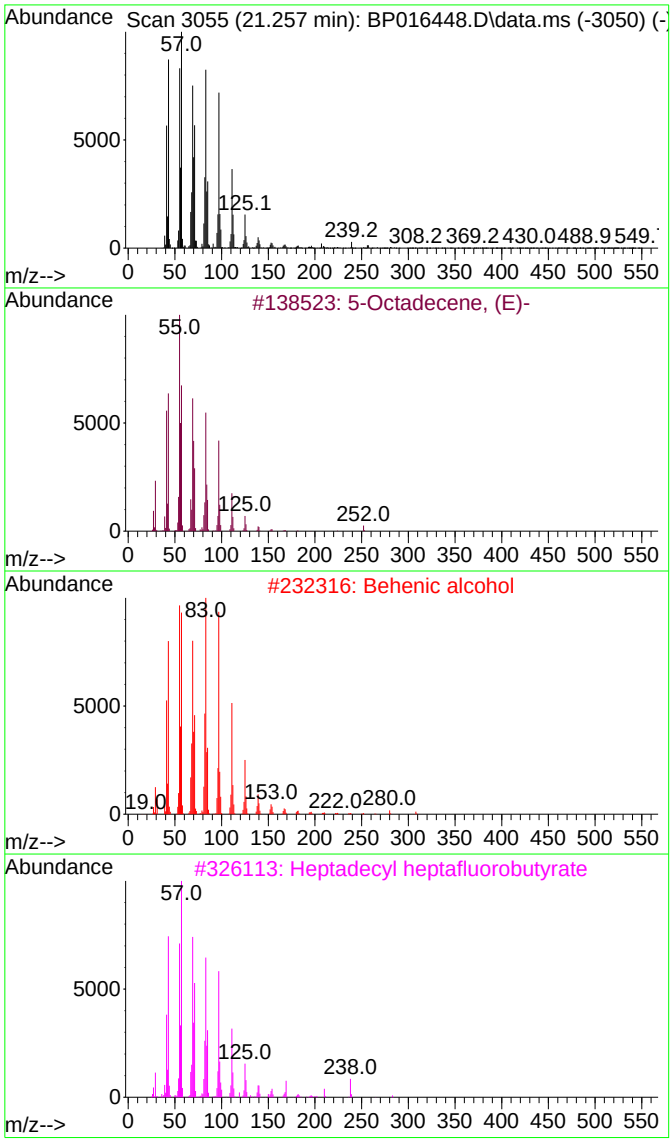
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

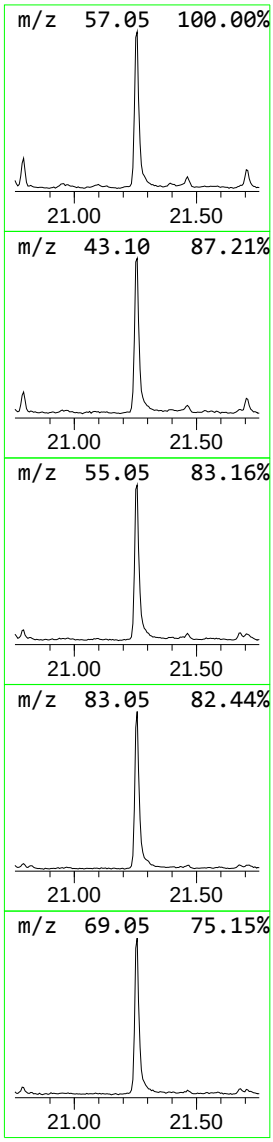
****

Peak Number 8 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	8.56 ng	2746150	Chrysene-d12	21.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Cyclotetradecane	196	C14H28	000295-17-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

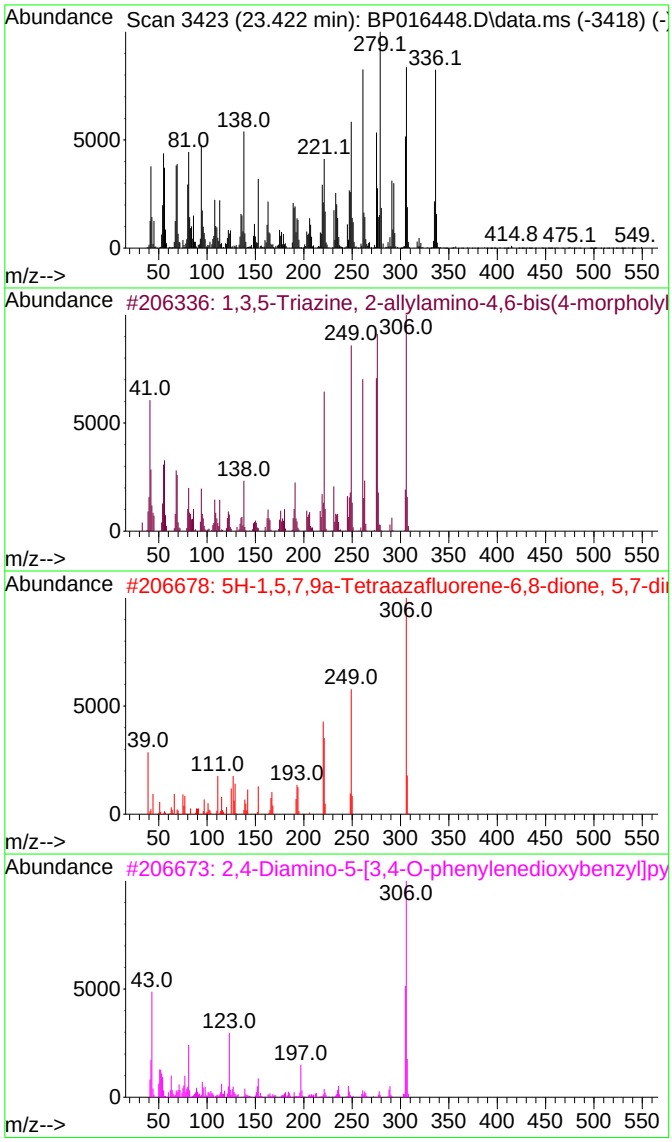
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

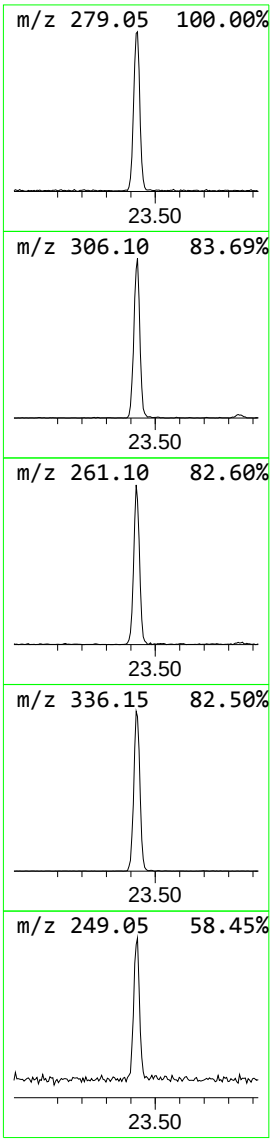
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,3,5-Triazine, 2-allylamin... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.422	3.74 ng	1065610	Perylene-d12	24.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine, 2-allylamino-4,6...	306	C14H22N6O2	332409-13-9	80
2	5H-1,5,7,9a-Tetraazafluorene-6,8...	306	C17H14N4O2	1000310-72-9	25
3	2,4-Diamino-5-[3,4-O-phenylenedi...	306	C17H14N4O2	071525-20-7	25
4	3-Carbethoxy-7-hydroxycoumarin, TMS	306	C15H18O5Si	1000511-83-6	25
5	Acetic acid, N'-[4,6-di(4-morpho...	337	C14H23N7O3	1000319-08-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080123\
Data File : BP016448.D
Acq On : 01 Aug 2023 10:31
Operator : MA/JU
Sample : 03767-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MMC-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP072723.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
3(5)-[[1,2-Dihy...	7.028	2.8	ng	440208	1	8.081	3099460	20.0
Ethanol, 2-(2-e...	7.658	2.6	ng	408681	1	8.081	3099460	20.0
2,4,7,9-Tetrame...	13.587	33.2	ng	10089700	3	14.728	6082480	20.0
N-Cyclohexyl-N'...	14.928	4.1	ng	1252630	3	14.728	6082480	20.0
n-Hexadecanoic ...	18.345	8.8	ng	3171760	4	17.492	7198490	20.0
9-Octadecenoic ...	19.257	2.5	ng	895716	4	17.492	7198490	20.0
Octadecanoic acid	19.569	3.5	ng	1138330	5	21.592	6417090	20.0
5-Octadecene, (E)-	21.257	8.6	ng	2746150	5	21.592	6417090	20.0
1,3,5-Triazine,...	23.422	3.7	ng	1065610	6	24.192	5697470	20.0