LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028502.D
Acq On : 21 Jan 2021 23:33
Operator : CG/JU
Sample : M1157-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4

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-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.663	225	251	271	rBV10	9015	72961	3.88%	0.822%
2	5.540	394	400	409	rVB	282564	415036	22.10%	4.676%
3	7.175	671	678	689	rVB2	166758	300565	16.00%	3.387%
4	8.016	814	821	827	rBV	114322	172094	9.16%	1.939%
5	9.192	1013	1021	1028	rBV	365237	595193	31.69%	6.706%
6	10.833	1293	1300	1305	rBV	151194	244034	12.99%	2.750%
7	10.880	1305	1308	1319	rVB	17974	29980	1.60%	0.338%
8	12.451	1566	1575	1580	rBV	76671	131311	6.99%	1.480%
9	13.286	1709	1717	1723	rBV	863000	1256062	66.87%	14.152%
10	14.110	1852	1857	1863	rBV	34920	45036	2.40%	0.507%
11	14.657	1944	1950	1955	rBV2	216973	313920	16.71%	3.537%
12	14.698	1955	1957	1969	rVB	31813	43541	2.32%	0.491%
13	16.139	2196	2202	2208	rBV	713372	986677	52.53%	11.117%
14	16.874	2322	2327	2342	rBV	133708	186611	9.93%	2.103%
15	17.386	2408	2414	2421	rBV	254667	356118	18.96%	4.012%
16	18.262	2558	2563	2572	rBV	235125	317331	16.89%	3.575%
17	19.009	2687	2690	2695	rBV	14599	22388	1.19%	0.252%
18	19.521	2773	2777	2785	rBV	117354	165238	8.80%	1.862%
19	19.656	2796	2800	2807	rVB	77177	97054	5.17%	1.094%
20	19.792	2819	2823	2829	rVB2	22665	31606	1.68%	0.356%
21	19.980	2849	2855	2863	rBV	1416666	1878362	100.00%	21.164%
22	20.344	2913	2917	2921	rBV	58711	69313	3.69%	0.781%
23	21.215	3061	3065	3070	rBV	250481	279494	14.88%	3.149%
24	21.515	3111	3116	3122	rBV	327739	398230	21.20%	4.487%
25	23.797	3498	3504	3511	rVB2	202085	383772	20.43%	4.324%
26	24.409	3604	3608	3616	rVB2	42867	83350	4.44%	0.939%

Sum of corrected areas: 8875277

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ClientSampleId :
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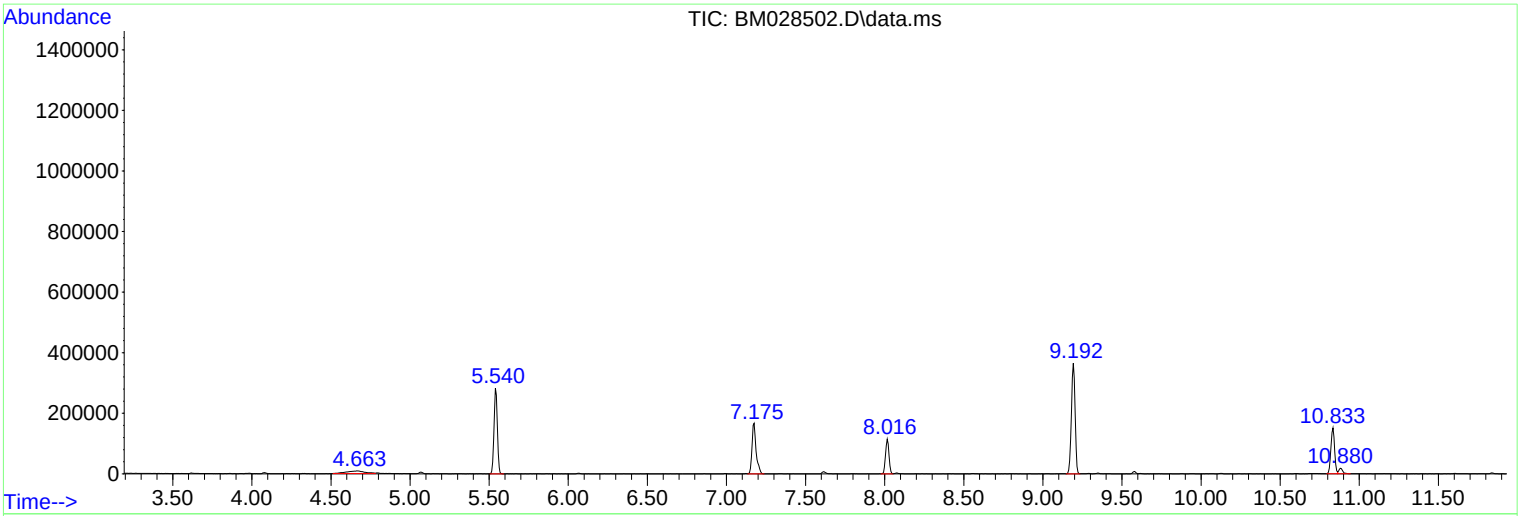
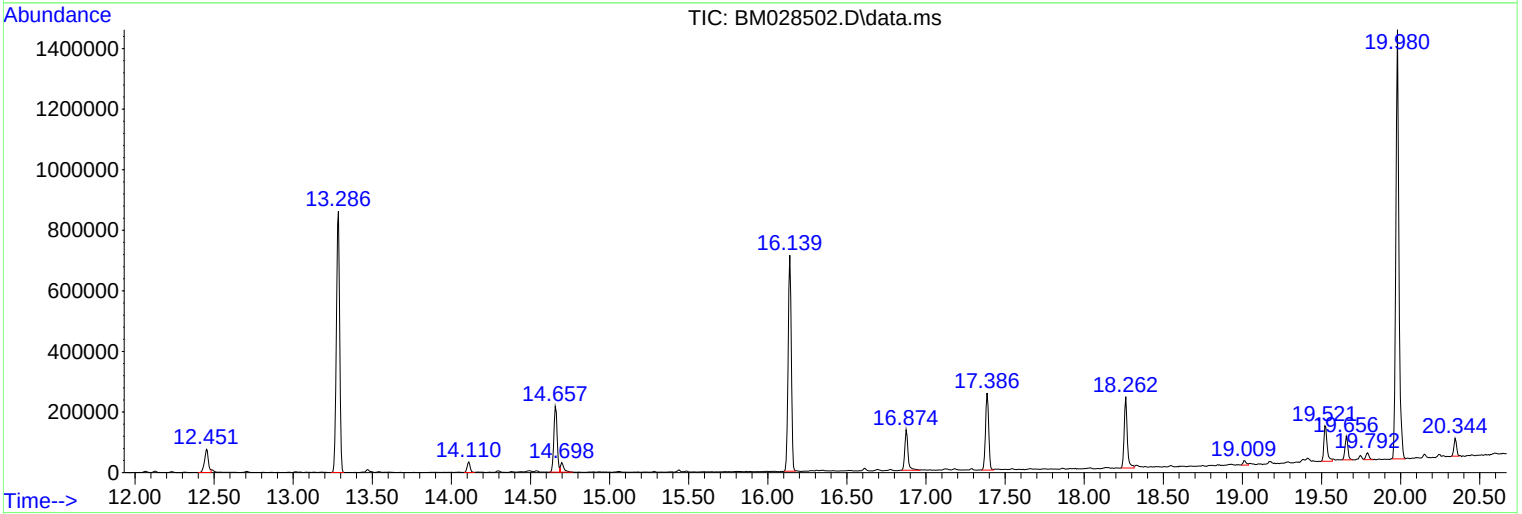
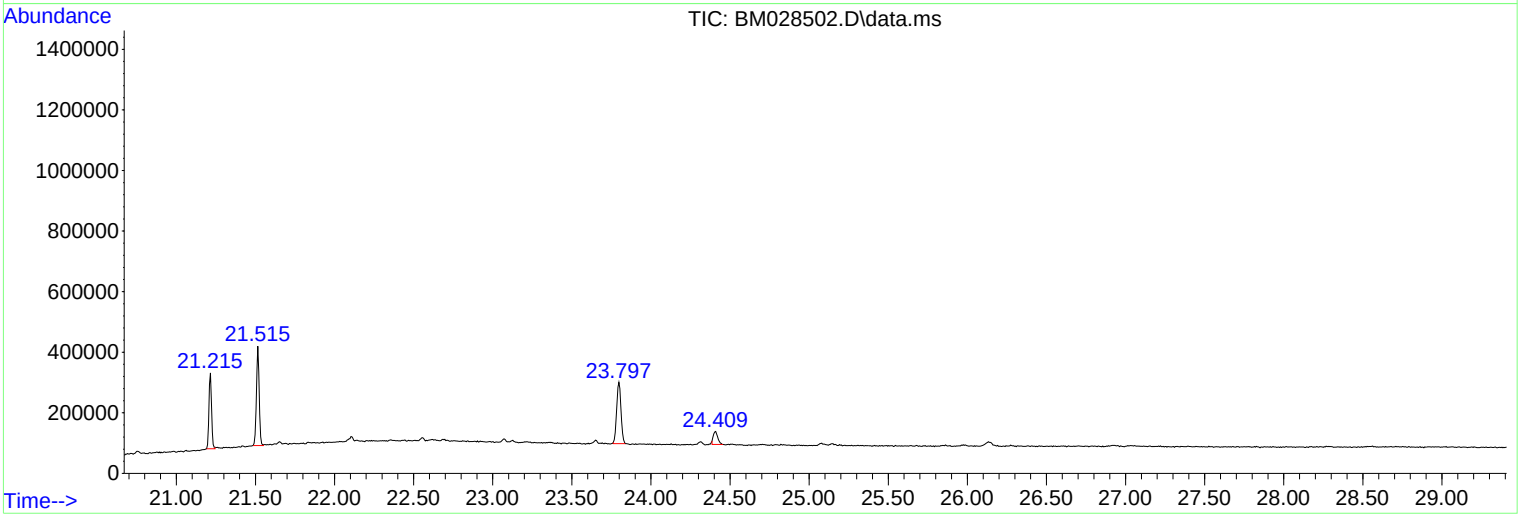
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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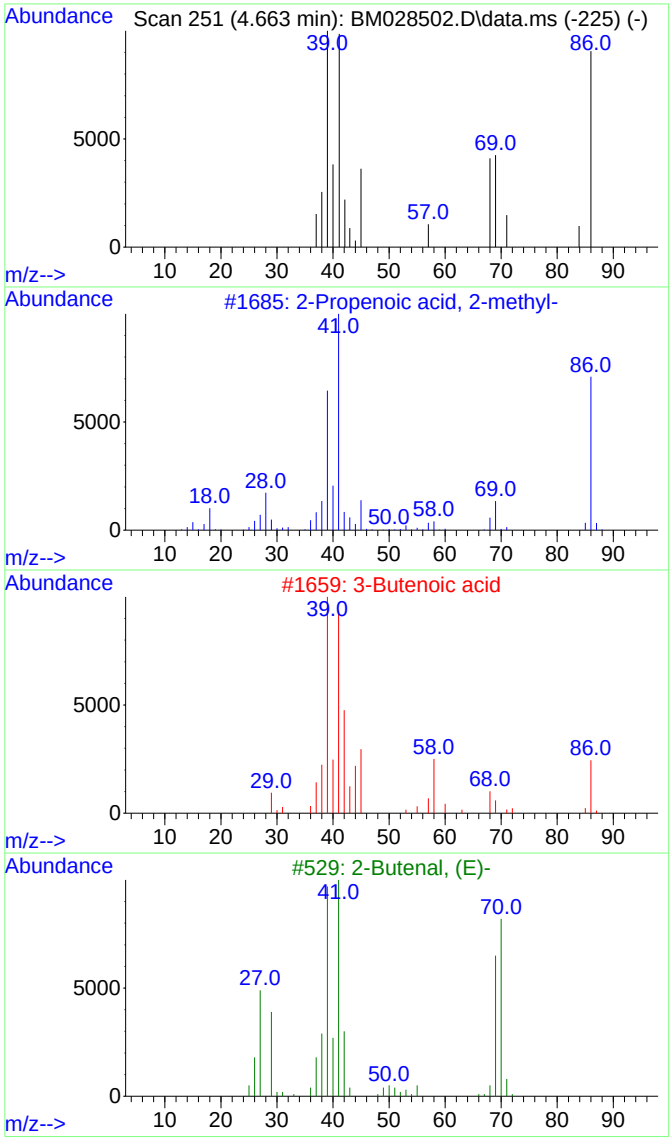
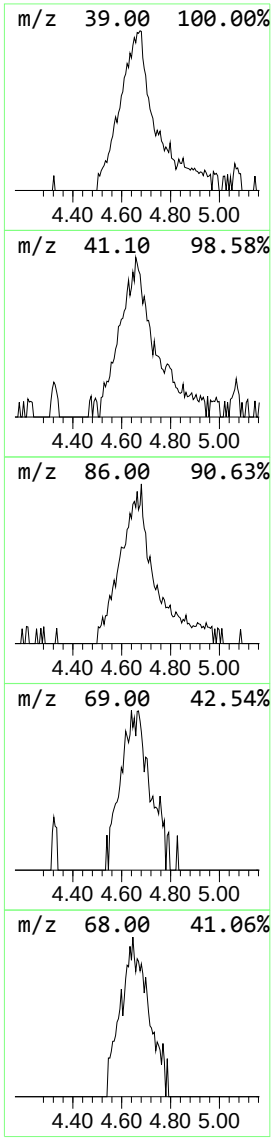
****
Peak Number 1 2-Propenoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.663	8.48 ng	72961	1,4-Dichlorobenzene-d4	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	72
2	3-Butenoic acid	86	C4H6O2	000625-38-7	72
3	2-Butenal, (E)-	70	C4H6O	000123-73-9	53
4	Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	50
5	2-Butenal	70	C4H6O	004170-30-3	45





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Instrument : BNA_M
ClientSampleId : MW-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

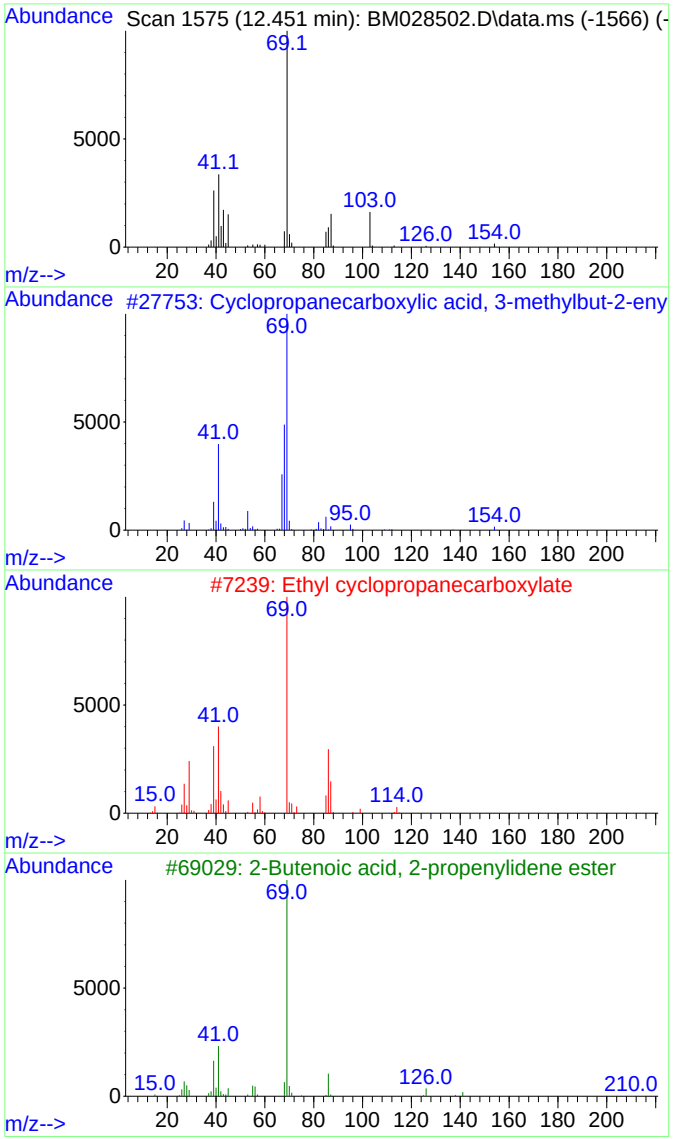
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

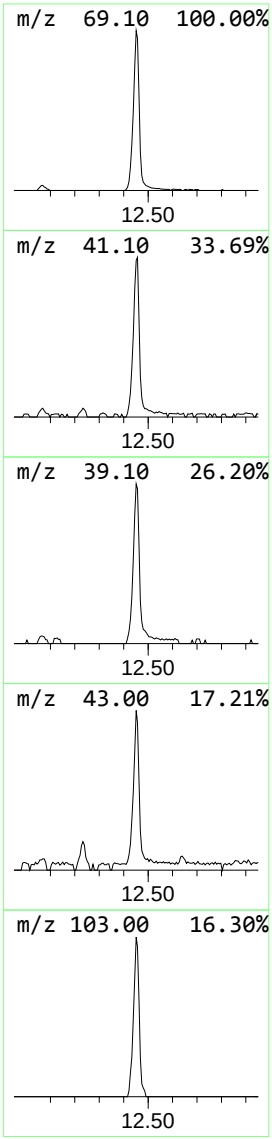
****

Peak Number 2 Cyclopropanecarboxylic acid... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	10.76 ng	131311	Naphthalene-d8	10.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	50
2	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	45
3	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
4	Oxazole	69	C3H3NO	000288-42-6	33
5	Isoxazole	69	C3H3NO	000288-14-2	9





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Instrument :
BNA_M
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
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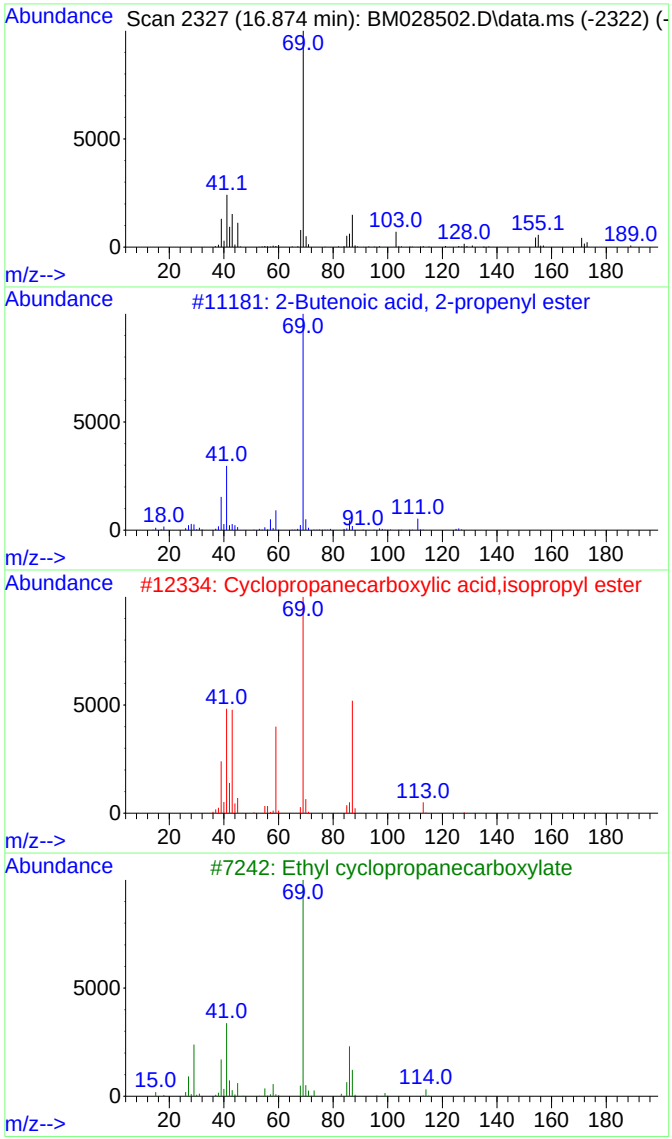
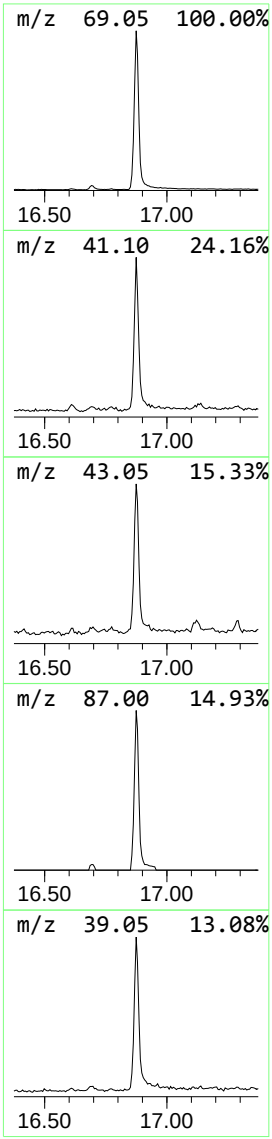
Peak Number 3 unknown16.874 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.874	10.48 ng	186611	Phenanthrene-d10	17.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenyl ester	126	C7H10O2	020474-93-5	40
2	Cyclopropanecarboxylic acid,isop...	128	C7H12O2	006887-83-8	38
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
4	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1000156-45-5	33
5	Cyclopropanecarboxylic acid chlo...	104	C4H5ClO	004023-34-1	9





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Instrument :
BNA_M
ClientSampleId :
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

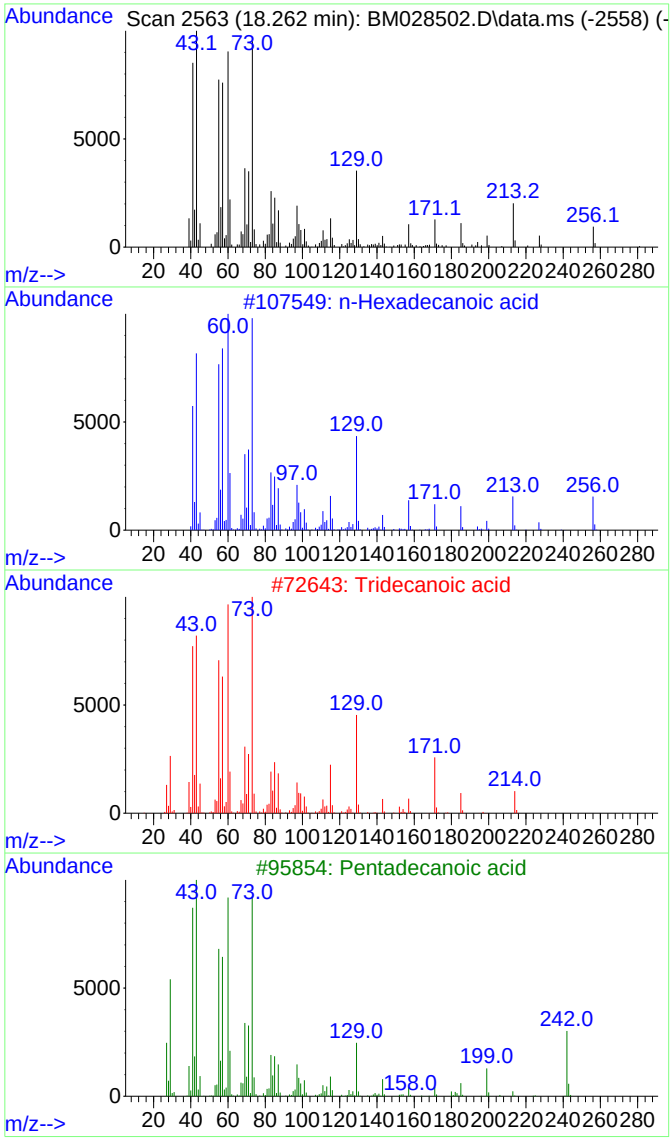
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

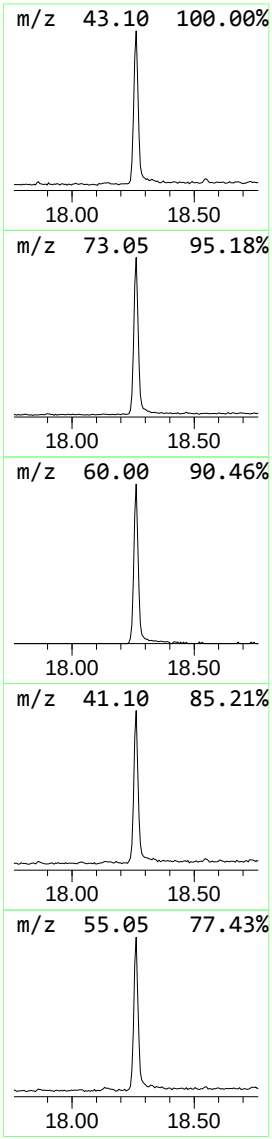
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.262	17.82 ng	317331	Phenanthrene-d10	17.386

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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Operator : CG/JU
Sample : M1157-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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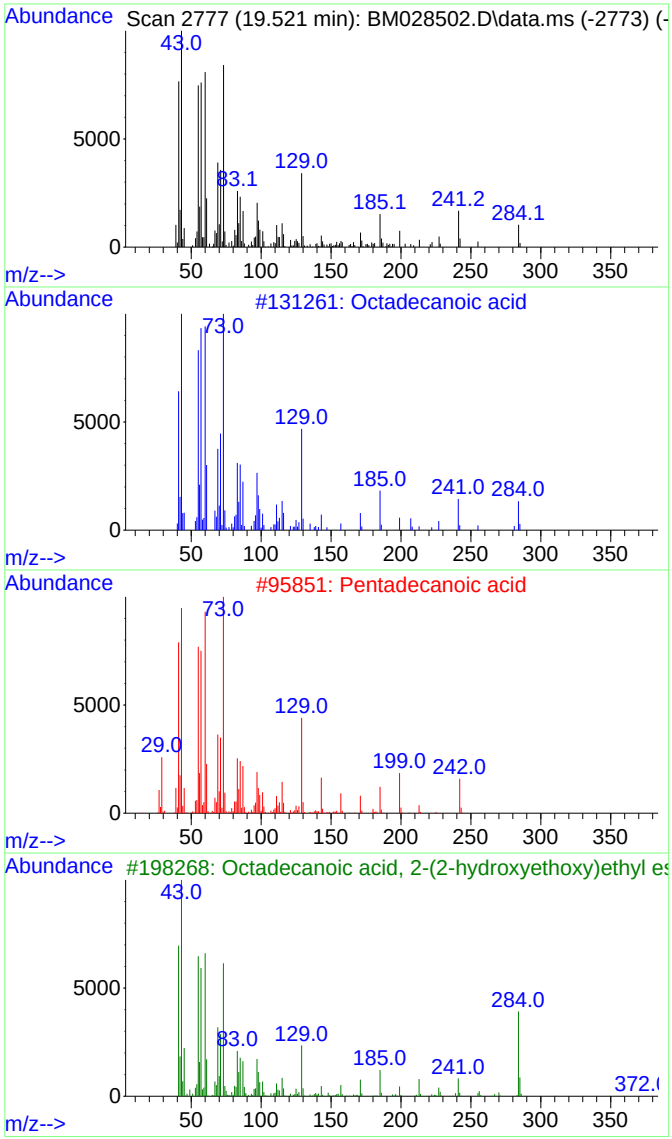
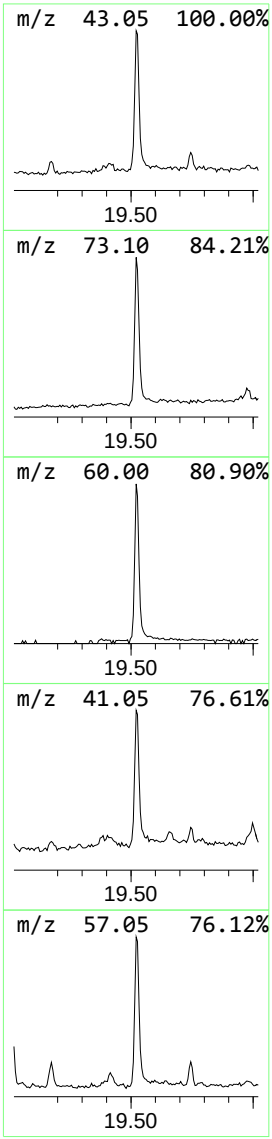
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.521	8.30 ng	165238	Chrysene-d12	21.515

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	94
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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Instrument : BNA_M
ClientSampleId : MW-4

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TIC Library : C:\DATABASE\NIST11.L
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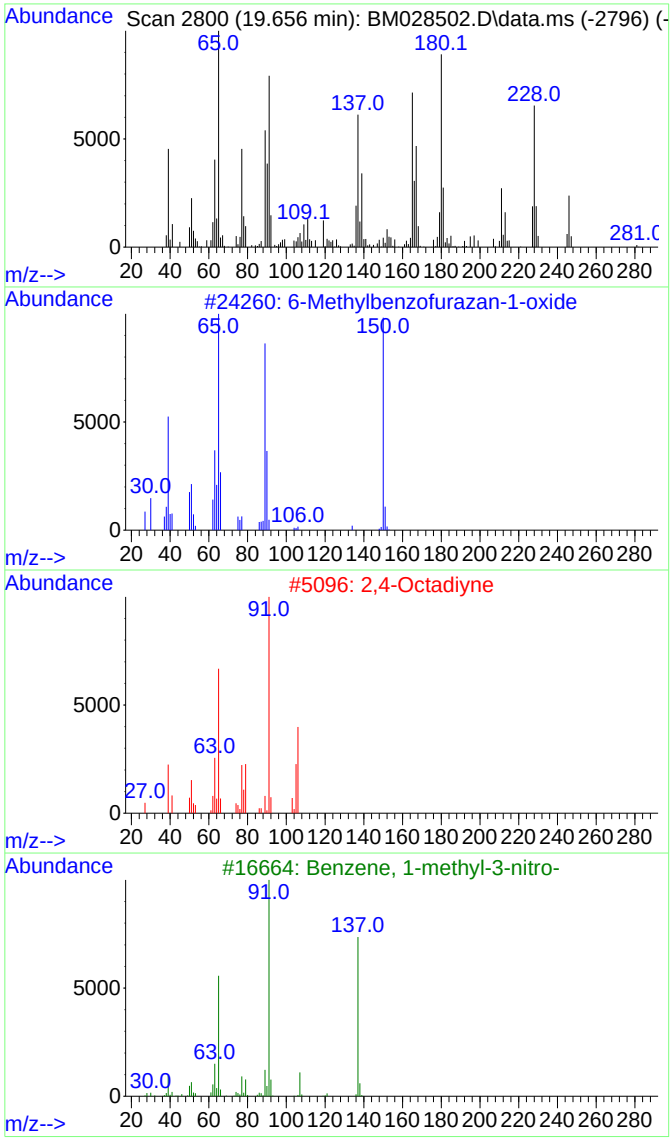
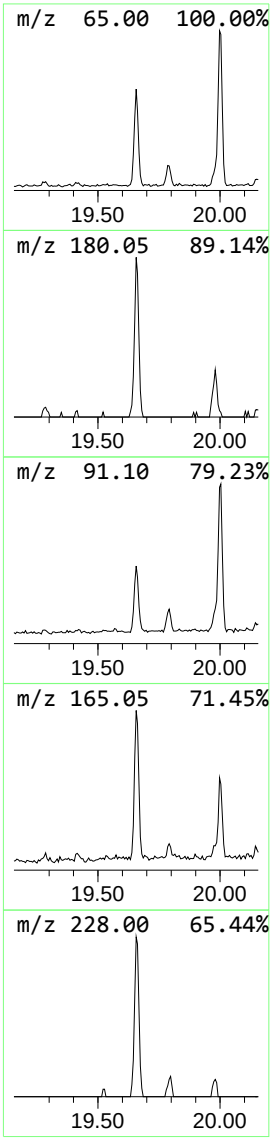
Peak Number 6 6-Methylbenzofurazan-1-oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.656	4.87 ng	97054	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methylbenzofurazan-1-oxide	150	C7H6N2O2	1000289-15-0	58
2	2,4-Octadiyne	106	C8H10	002809-71-4	53
3	Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	50
4	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	50
5	Benzoic acid, 4-nitro-	167	C7H5NO4	000062-23-7	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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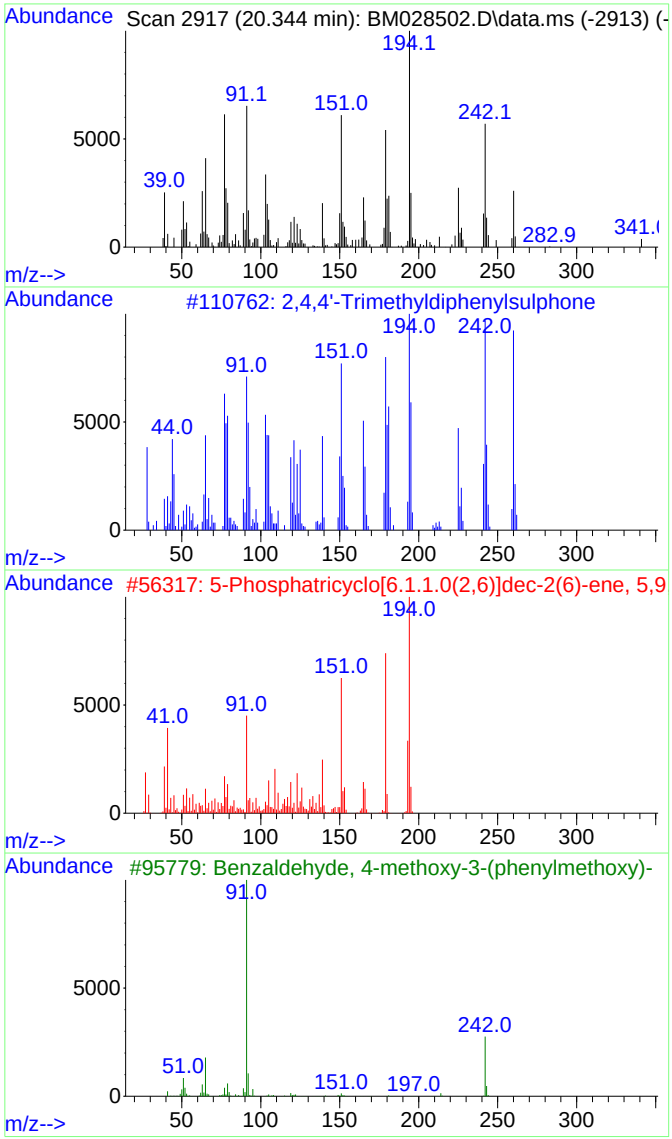
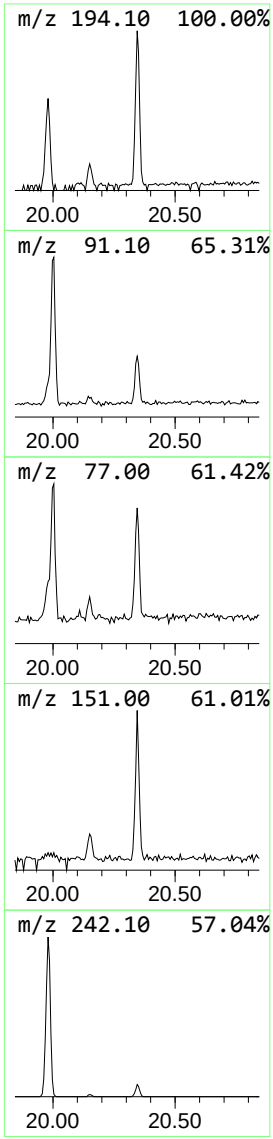
****
Peak Number 7 2,4,4'-Trimethyldiphenylsul... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.344	3.48 ng	69313	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4'-Trimethyldiphenylsulphone	260	C15H16O2S	013249-97-3	83
2	5-Phosphatricyclo[6.1.1.0(2,6)]d...	194	C12H19P	1000151-12-3	38
3	Benzaldehyde, 4-methoxy-3-(pheny...	242	C15H14O3	006346-05-0	35
4	.alpha.-hydroxy-3,4-methylenedio...	194	C10H10O4	1000378-94-3	35
5	1,6-Heptadien-3-yne, 5-methyl-	106	C8H10	1000142-71-3	30





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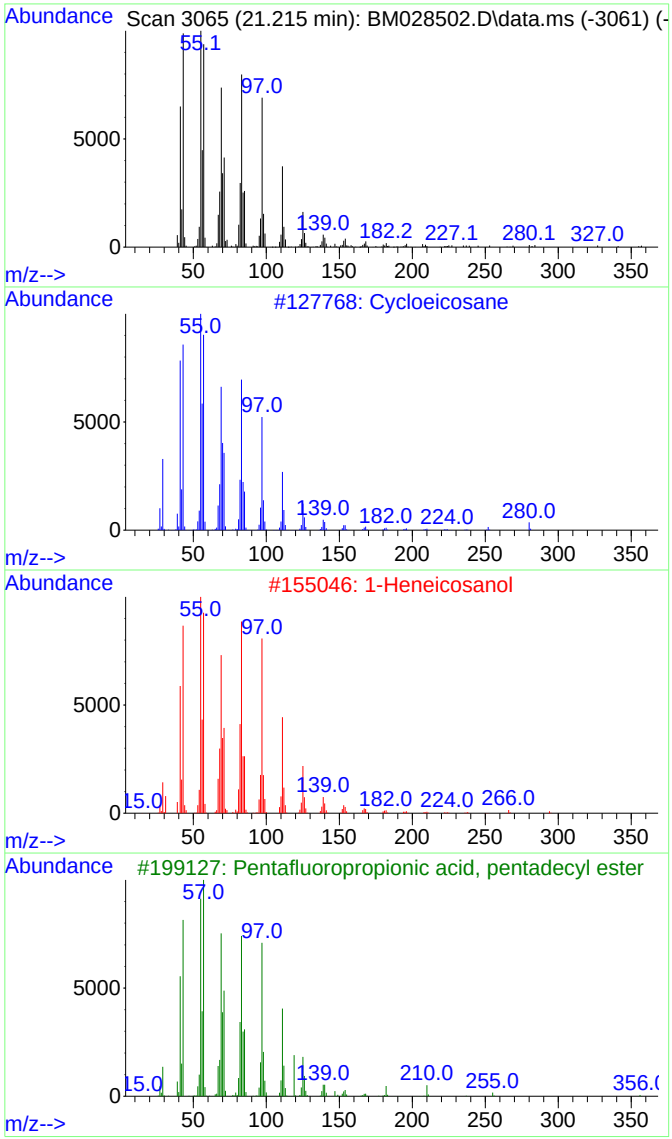
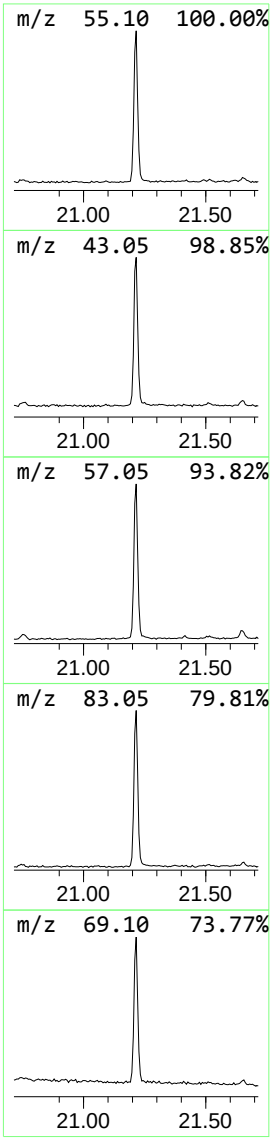
Peak Number 8 Cycloeicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.215	14.04 ng	279494	Chrysene-d12	21.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Cyclotetracosane	336	C24H48	000297-03-0	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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Instrument : BNA_M
ClientSampleId : MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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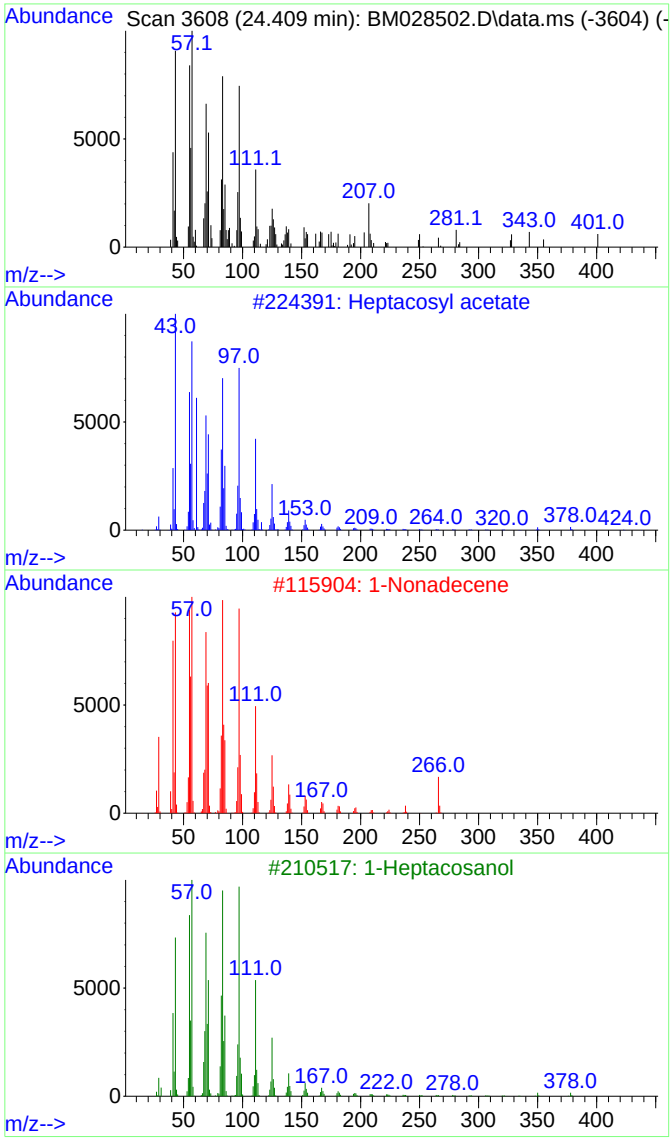
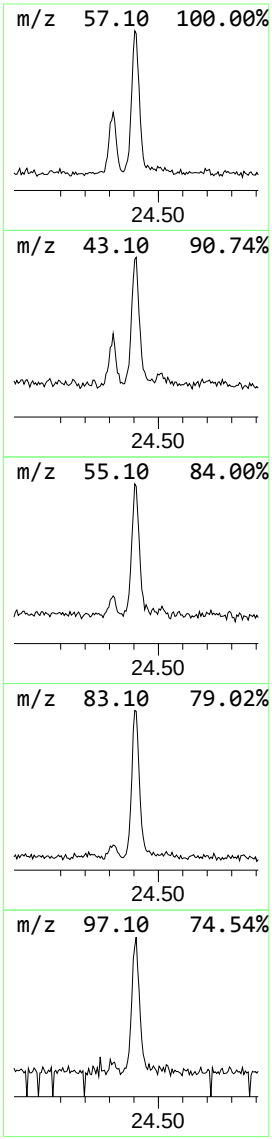
Peak Number 9 Heptacosyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.409	4.34 ng	83350	Perylene-d12	23.797

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	87
2	1-Nonadecene	266	C19H38	018435-45-5	83
3	1-Heptacosanol	396	C27H56O	002004-39-9	81
4	Octacosanol	410	C28H58O	000557-61-9	76
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	76





Tentatively Identified Compound (LSC) summary

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Sample : M1157-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Propenoic aci...	4.663	8.5	ng	72961	1	8.016	172094	20.0
Cyclopropanecar...	12.451	10.8	ng	131311	2	10.833	244034	20.0
unknown16.874	16.874	10.5	ng	186611	4	17.386	356118	20.0
n-Hexadecanoic ...	18.262	17.8	ng	317331	4	17.386	356118	20.0
Octadecanoic acid	19.521	8.3	ng	165238	5	21.515	398230	20.0
6-Methylbenzofu...	19.656	4.9	ng	97054	5	21.515	398230	20.0
2,4,4'-Trimethy...	20.344	3.5	ng	69313	5	21.515	398230	20.0
Cycloeicosane	21.215	14.0	ng	279494	5	21.515	398230	20.0
Heptacosyl acetate	24.409	4.3	ng	83350	6	23.797	383772	20.0