LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120321\
Data File : BM033296.D
Acq On : 03 Dec 2021 21:02
Operator : CG/JU
Sample : M4917-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-16R

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-BM112421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.119	128	133	140	rBV	66637	100595	1.33%	0.302%
2	5.048	286	291	298	rBV	173619	249203	3.29%	0.749%
3	5.519	364	371	378	rBV	1072066	1636315	21.63%	4.917%
4	7.107	633	641	660	rBV	657909	1200773	15.87%	3.608%
5	7.925	771	780	787	rBV	524380	866154	11.45%	2.603%
6	9.089	969	978	986	rBV	1646203	2765644	36.55%	8.311%
7	10.495	1211	1217	1231	rBV	158312	293297	3.88%	0.881%
8	10.725	1246	1256	1263	rBV	651441	1139168	15.06%	3.423%
9	13.171	1665	1672	1685	rVB	3453223	5165713	68.27%	15.523%
10	13.366	1700	1705	1708	rBV	54559	79320	1.05%	0.238%
11	13.442	1714	1718	1724	rVB	89451	136931	1.81%	0.411%
12	14.183	1840	1844	1856	rBV3	73804	129474	1.71%	0.389%
13	14.548	1900	1906	1918	rVB	911508	1403861	18.55%	4.219%
14	15.130	1998	2005	2010	rBV	55769	154800	2.05%	0.465%
15	16.036	2153	2159	2166	rBV	2401827	3422597	45.23%	10.285%
16	17.195	2353	2356	2362	rVB3	65605	83179	1.10%	0.250%
17	17.289	2366	2372	2378	rVV	1110063	1594534	21.07%	4.791%
18	17.948	2480	2484	2489	rVB	139548	173896	2.30%	0.523%
19	18.171	2518	2522	2531	rBV	208757	327415	4.33%	0.984%
20	19.118	2679	2683	2693	rVB	202557	278365	3.68%	0.836%
21	19.900	2810	2816	2823	rVB	5930837	7566287	100.00%	22.736%
22	21.147	3024	3028	3037	rVB2	564729	733385	9.69%	2.204%
23	21.224	3038	3041	3045	rBV	141950	157586	2.08%	0.474%
24	21.447	3075	3079	3087	rBV	1345576	1765429	23.33%	5.305%
25	23.783	3470	3476	3484	rVB2	936738	1854626	24.51%	5.573%

Sum of corrected areas: 33278547

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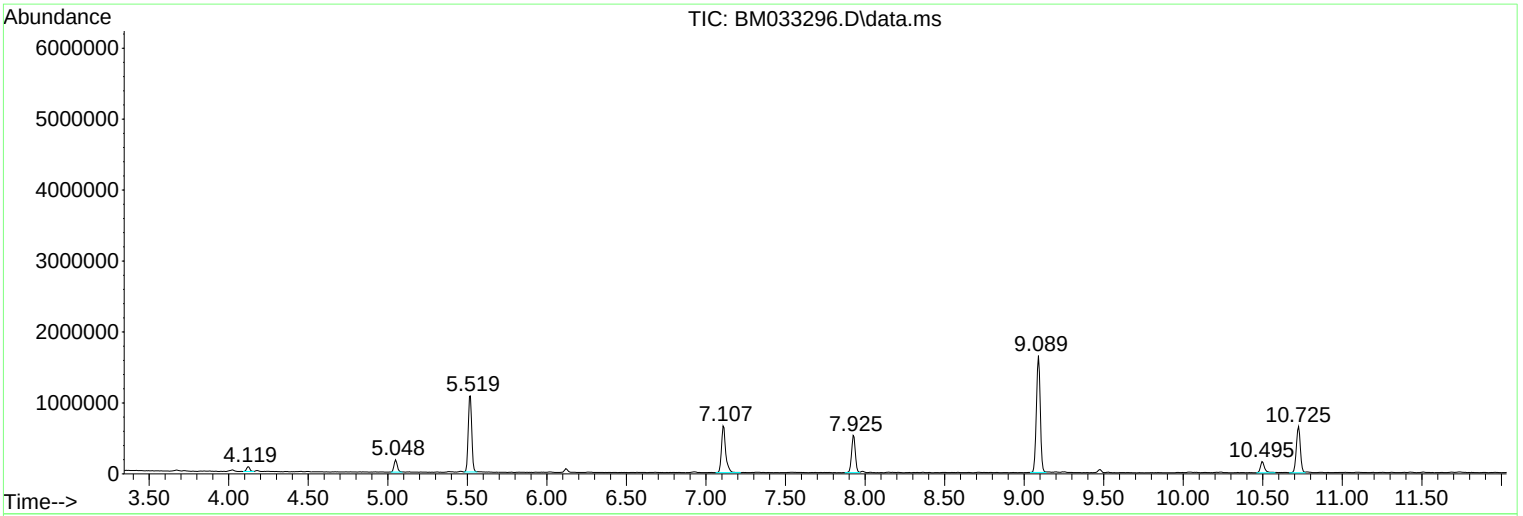
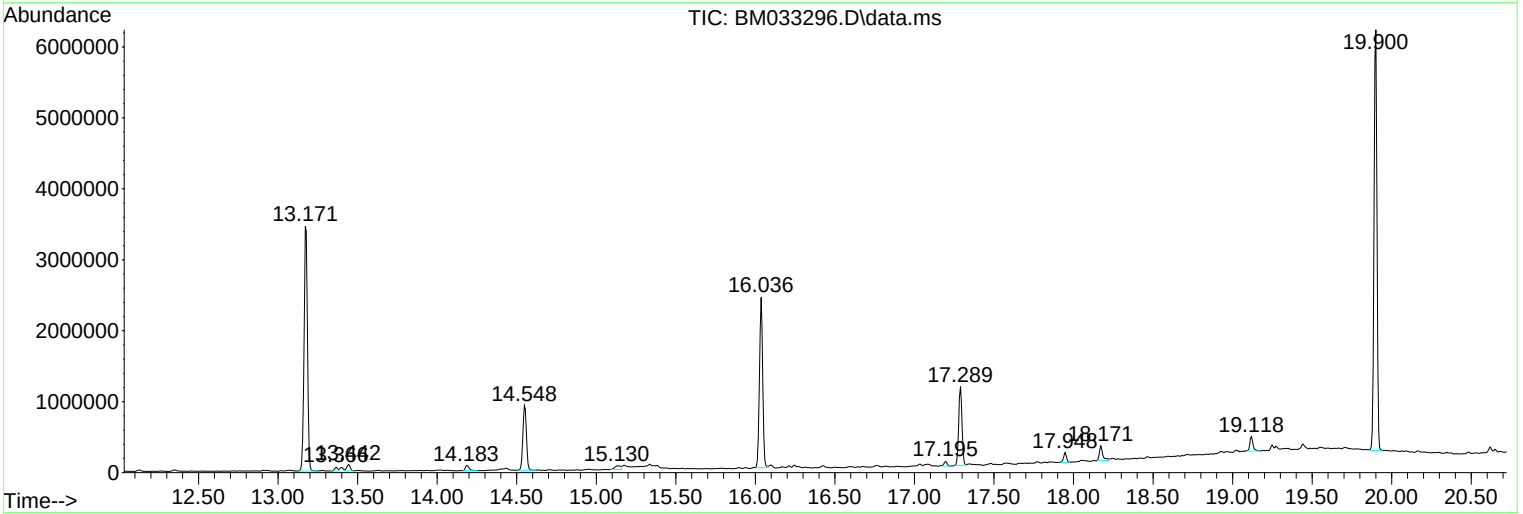
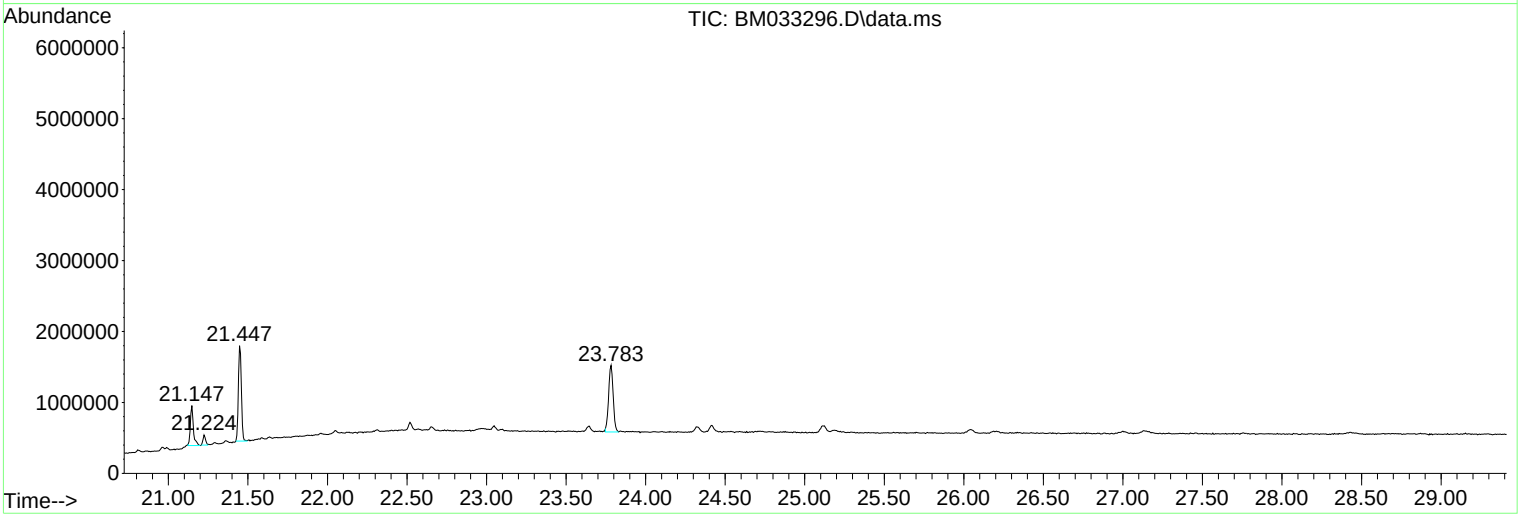
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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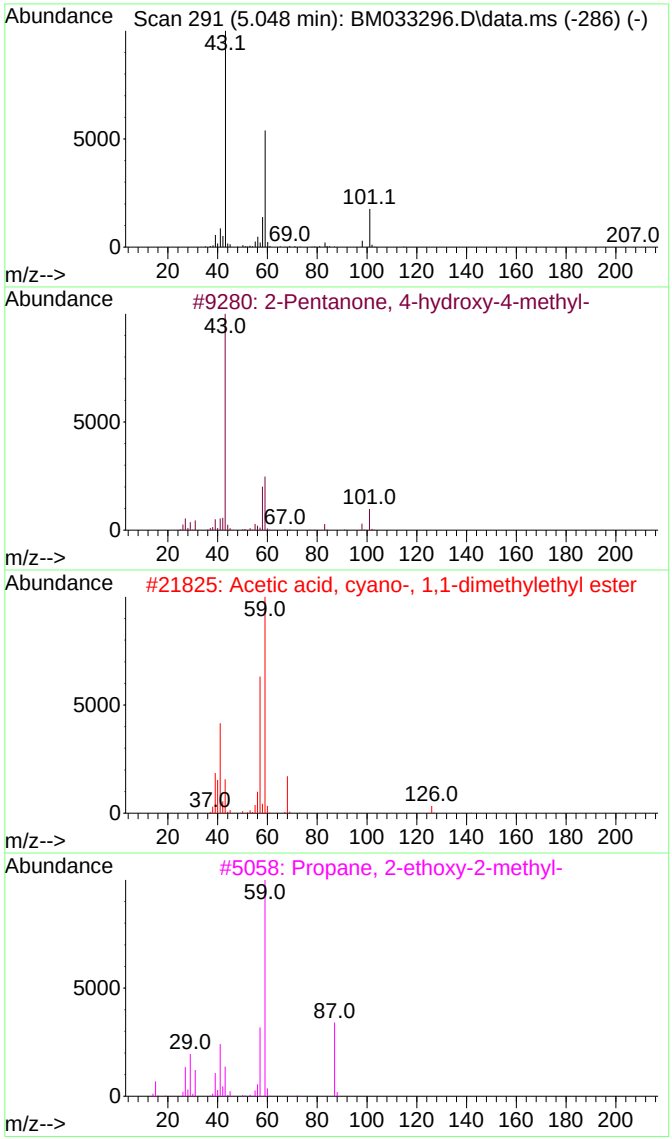
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

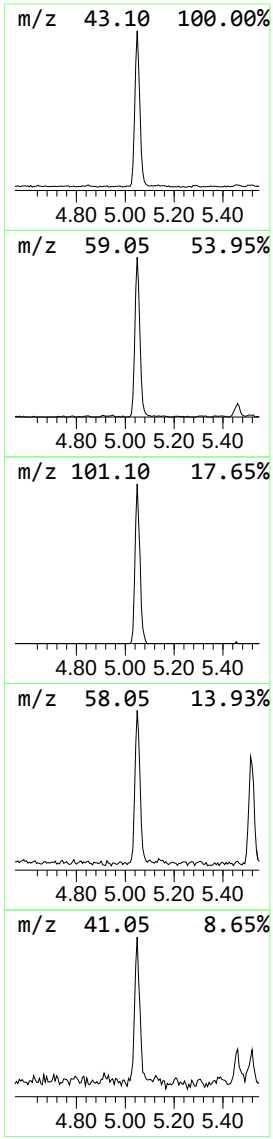
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.048	5.75 ng	249203	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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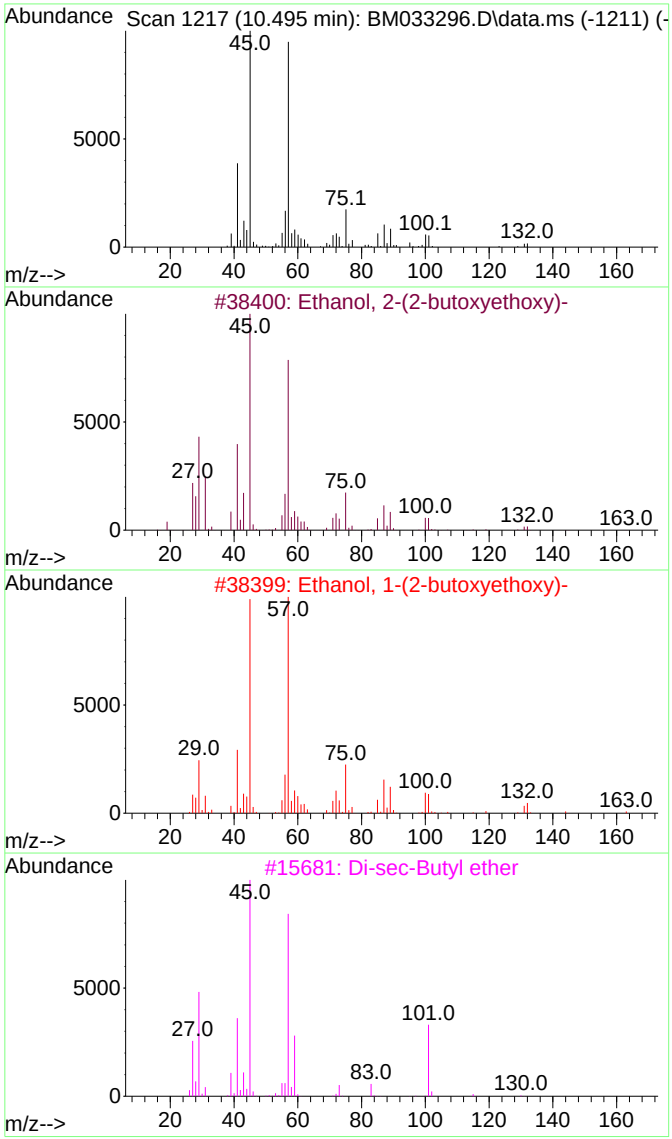
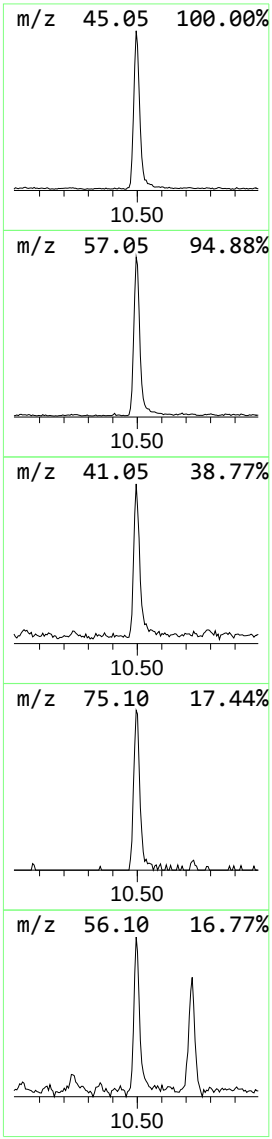
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.495	5.15 ng	293297	Naphthalene-d8	10.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-16R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
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TIC Library : C:\Database\NIST20.L
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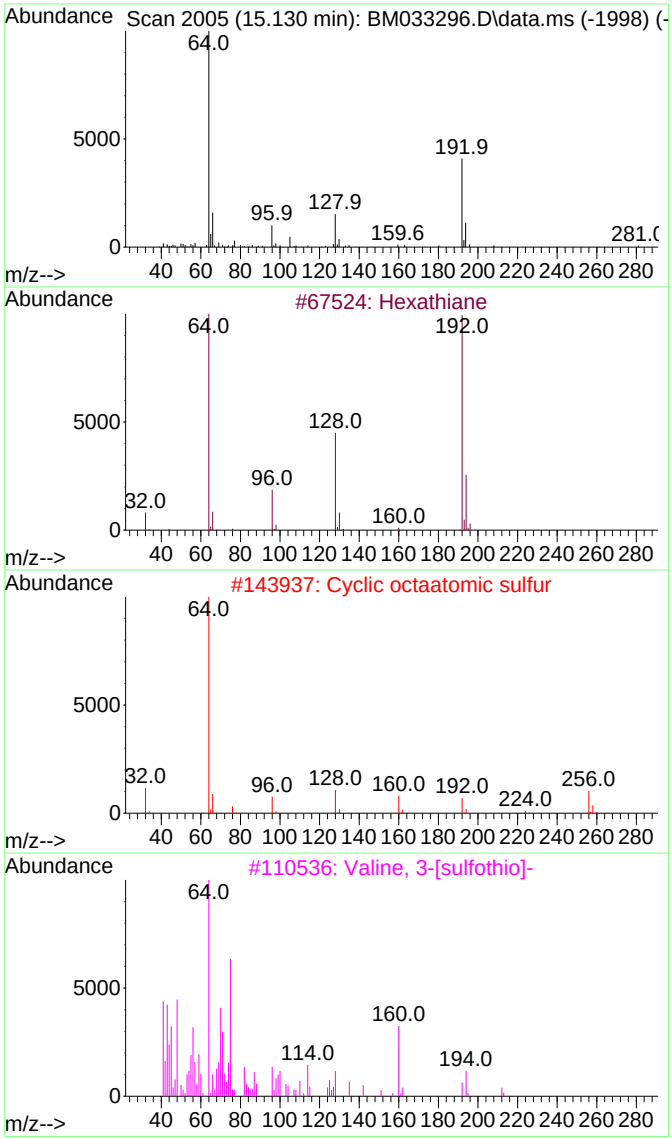
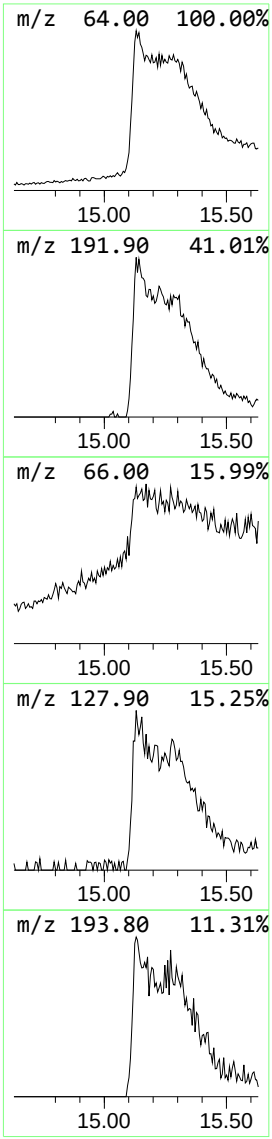
****

Peak Number 4 Hexathiane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.130	2.21 ng	154800	Acenaphthene-d10	14.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	Cyclic octaatomic sulfur	256	S8	010544-50-0	40
3	Valine, 3-[sulfothio]-	229	C5H11NO5S2	055631-63-5	9
4	Ethyl Chloride	64	C2H5Cl	000075-00-3	7
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5





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BNA_M
ClientSampleId :
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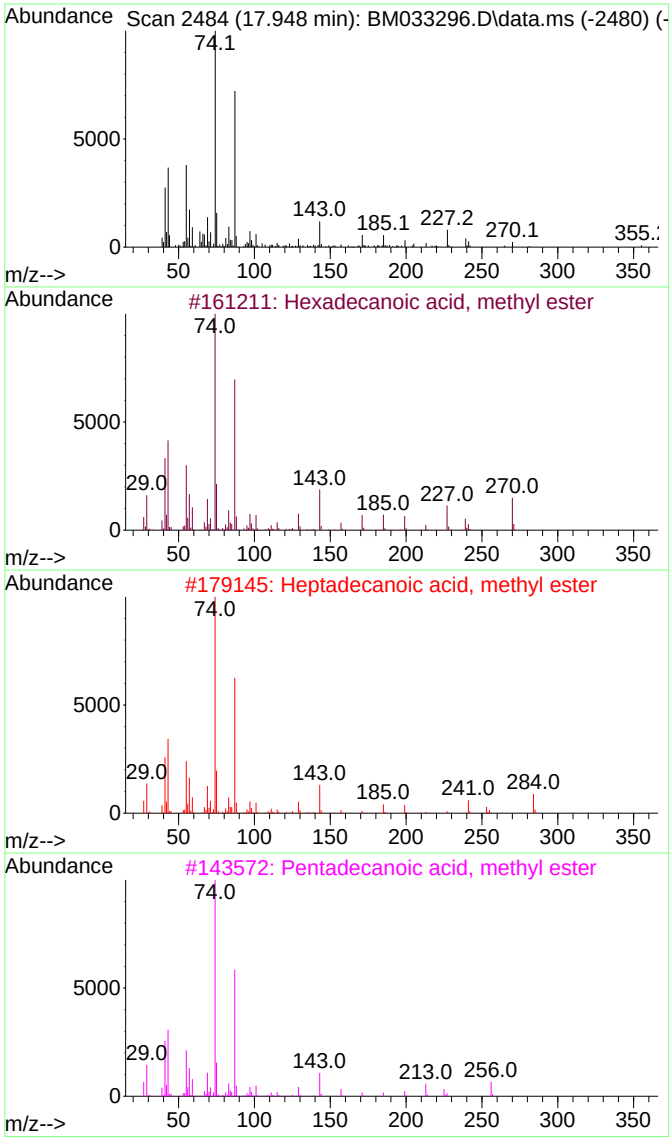
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

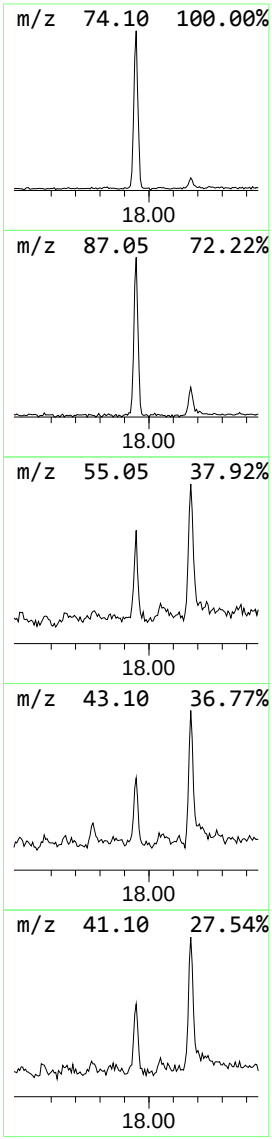
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.948	2.18 ng	173896	Phenanthrene-d10	17.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	92
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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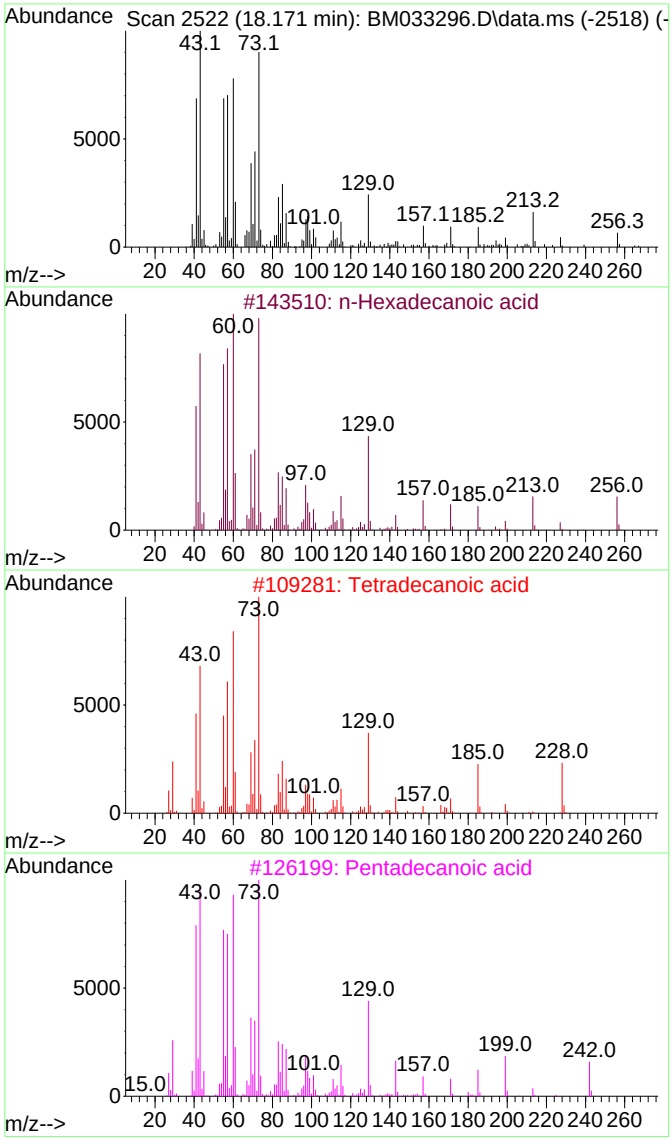
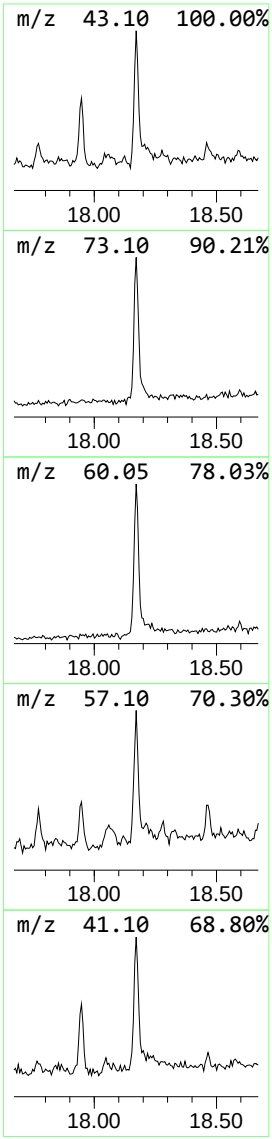
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.171	4.11 ng	327415	Phenanthrene-d10	17.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	62
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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TIC Library : C:\Database\NIST20.L
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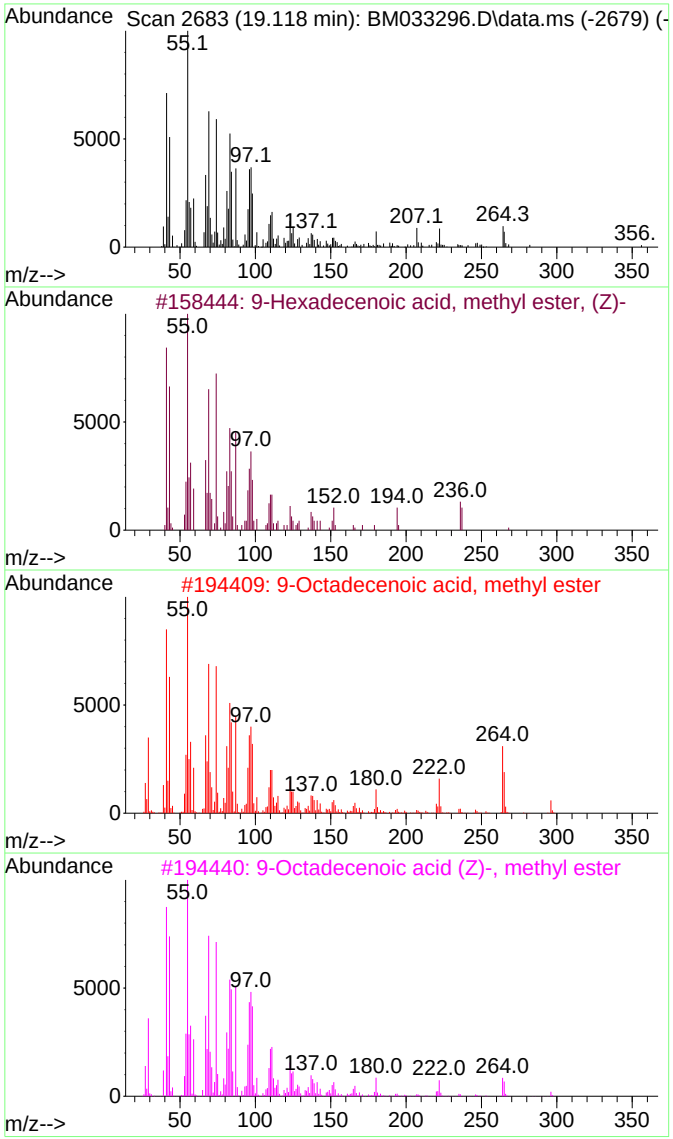
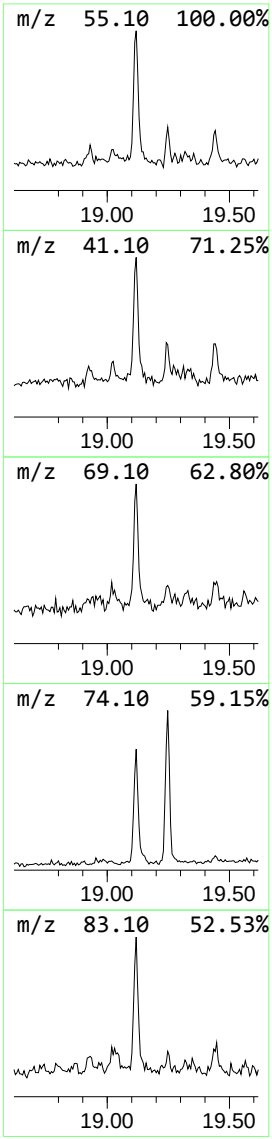
****
Peak Number 7 9-Hexadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.118	3.49 ng	278365	Phenanthrene-d10	17.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	94
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	94
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	93
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	93





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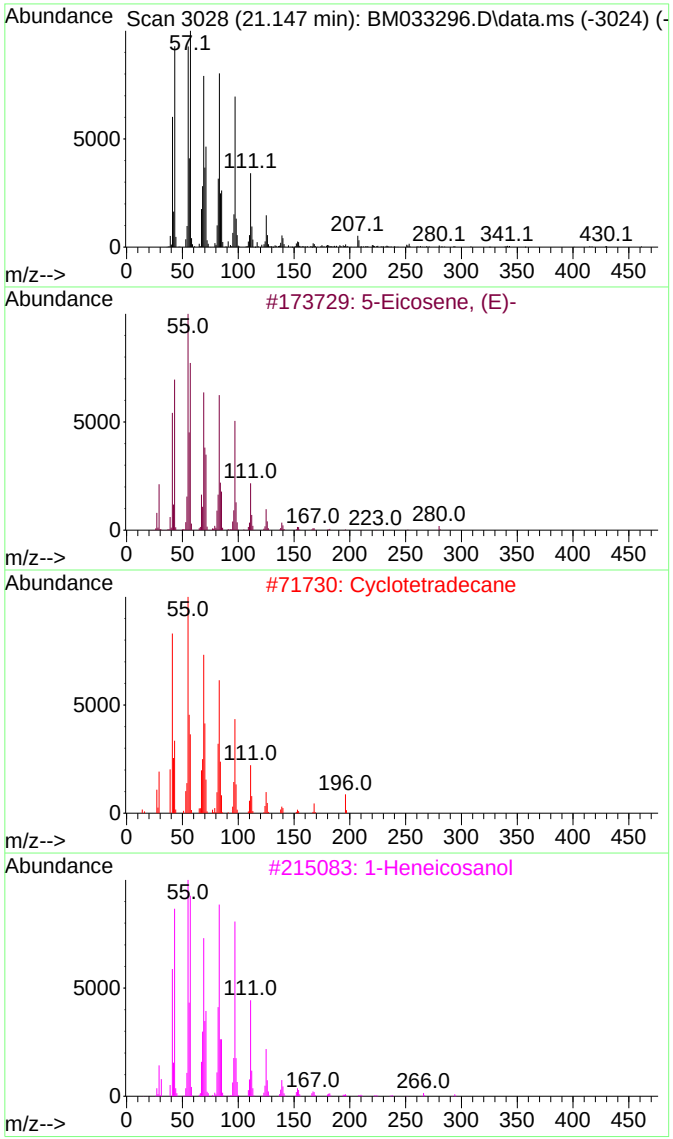
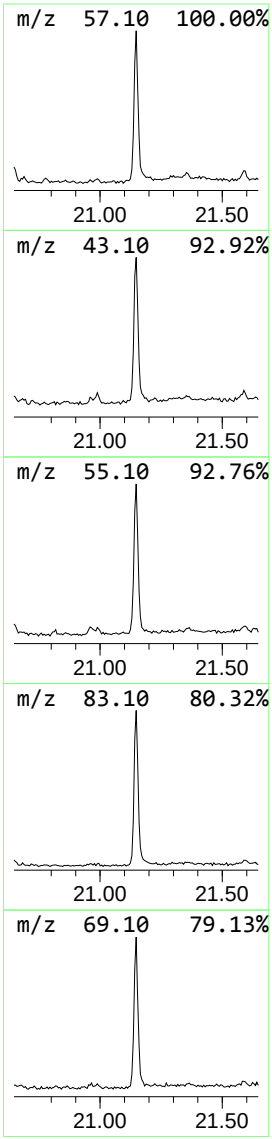
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.147	8.31 ng	733385	Chrysene-d12	21.447

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Cyclotetradecane	196	C14H28	000295-17-0	96
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.048	5.8	ng	249203	1	7.925	866154	20.0
Ethanol, 2-(2-b...	10.495	5.2	ng	293297	2	10.725	1139170	20.0
Hexathiane	15.130	2.2	ng	154800	3	14.548	1403860	20.0
Hexadecanoic ac...	17.948	2.2	ng	173896	4	17.289	1594530	20.0
n-Hexadecanoic ...	18.171	4.1	ng	327415	4	17.289	1594530	20.0
9-Hexadecenoic ...	19.118	3.5	ng	278365	4	17.289	1594530	20.0
5-Eicosene, (E)-	21.147	8.3	ng	733385	5	21.447	1765430	20.0