LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112120\
Data File : BP004047.D
Acq On : 21 Nov 2020 20:21
Operator : CG/JU
Sample : L4839-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B5-7-8

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-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.917	3	5	24	rVB	4772742	5938355	100.00%	21.552%
2	3.076	26	32	42	rVB	58057	119001	2.00%	0.432%
3	3.164	42	47	53	rBV	169112	238455	4.02%	0.865%
4	4.628	291	296	311	rVB	153197	220652	3.72%	0.801%
5	5.264	399	404	413	rBV	162359	230328	3.88%	0.836%
6	5.805	488	496	511	rBV	1246989	1963359	33.06%	7.126%
7	7.452	769	776	789	rBV	1181427	2077355	34.98%	7.539%
8	7.840	835	842	850	rBV	41145	71167	1.20%	0.258%
9	8.263	903	914	921	rBV	415774	664114	11.18%	2.410%
10	9.428	1104	1112	1120	rBV	755070	1248331	21.02%	4.531%
11	11.093	1388	1395	1409	rBV	503279	859753	14.48%	3.120%
12	13.510	1799	1806	1817	rBV	1685616	2452774	41.30%	8.902%
13	14.310	1937	1942	1949	rBV	143959	203252	3.42%	0.738%
14	14.887	2030	2040	2048	rBV	779023	1148383	19.34%	4.168%
15	16.369	2286	2292	2308	rBV	1195938	1805766	30.41%	6.554%
16	17.616	2498	2504	2510	rBV	883270	1285051	21.64%	4.664%
17	18.463	2644	2648	2655	rBV	271915	441609	7.44%	1.603%
18	18.892	2717	2721	2728	rBV	56615	78461	1.32%	0.285%
19	19.592	2837	2840	2846	rVB	50207	60454	1.02%	0.219%
20	19.669	2849	2853	2861	rBV	110669	189225	3.19%	0.687%
21	20.116	2924	2929	2935	rBV	2664591	3219633	54.22%	11.685%
22	21.310	3129	3132	3139	rBV4	100690	193110	3.25%	0.701%
23	21.651	3184	3190	3195	rBV	1086638	1455183	24.50%	5.281%
24	24.116	3602	3609	3617	rBV	684741	1389302	23.40%	5.042%

Sum of corrected areas: 27553073

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Misc :
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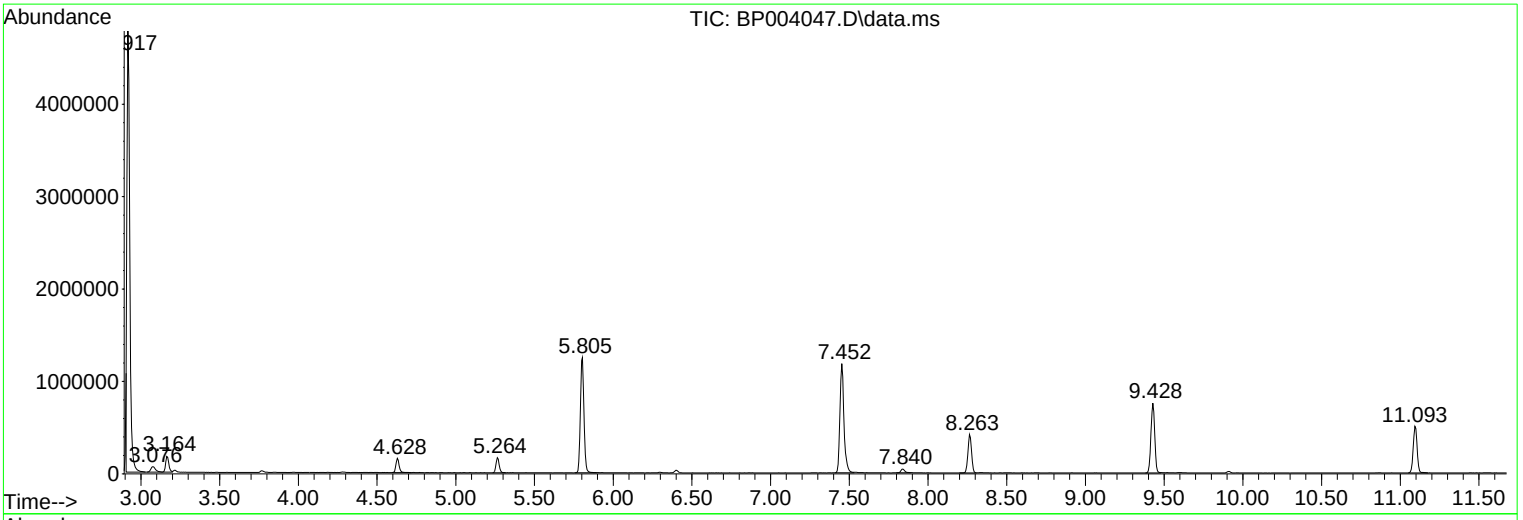
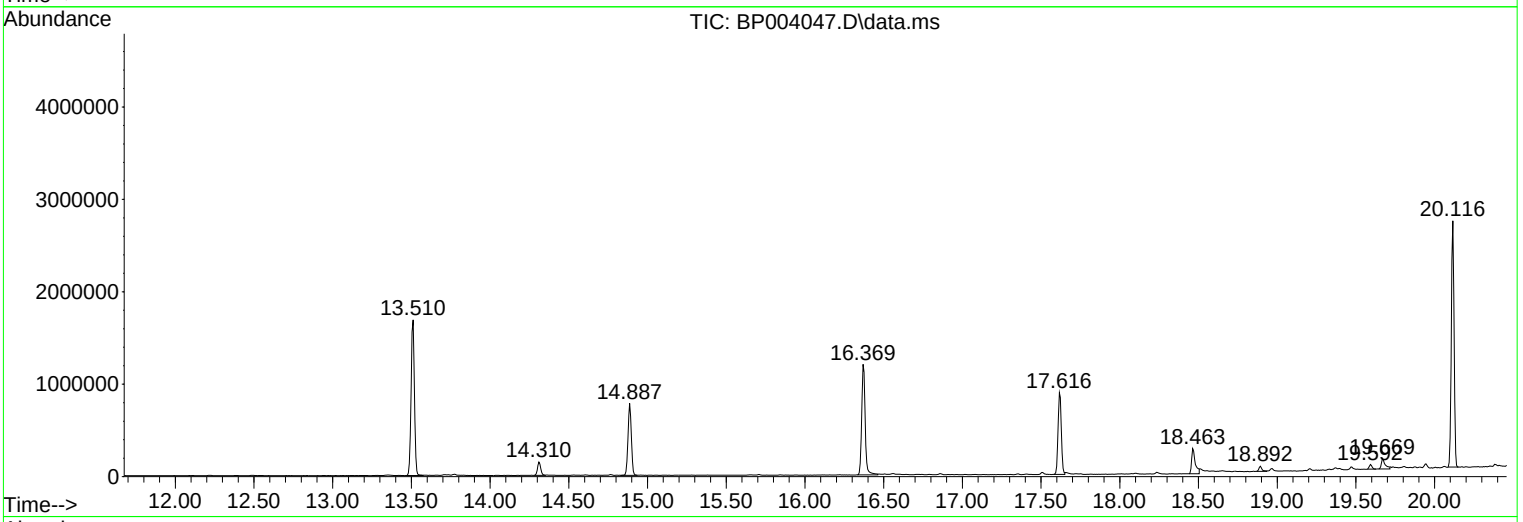
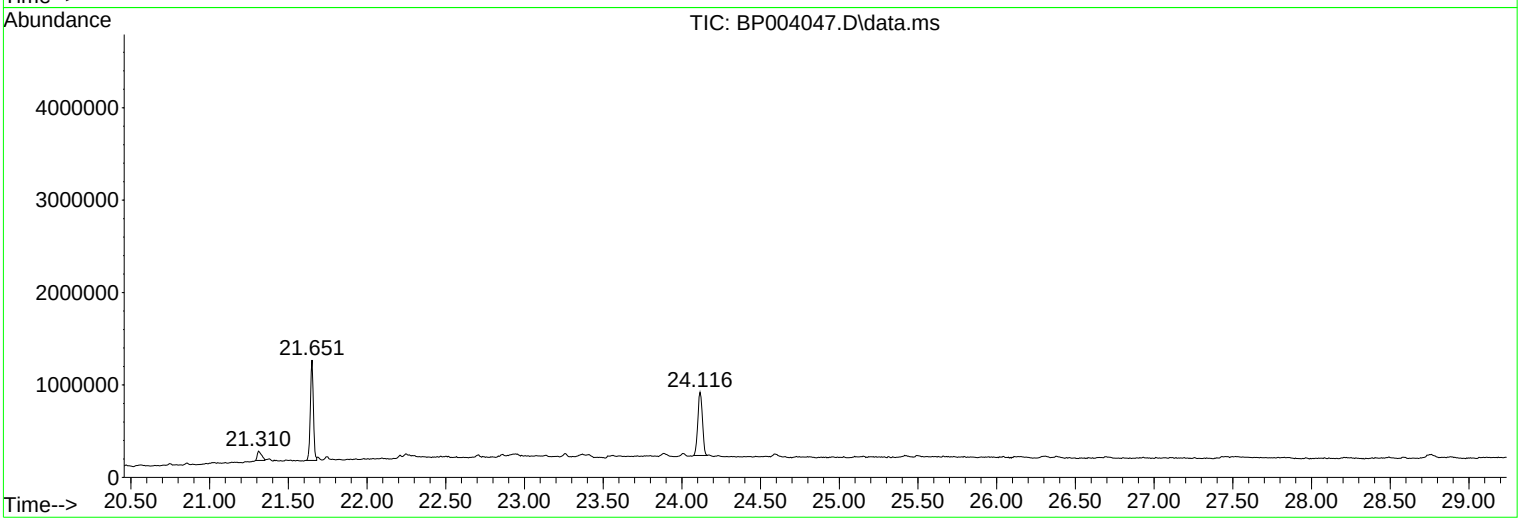
Instrument :
BNA_P
ClientSampleId :
B5-7-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.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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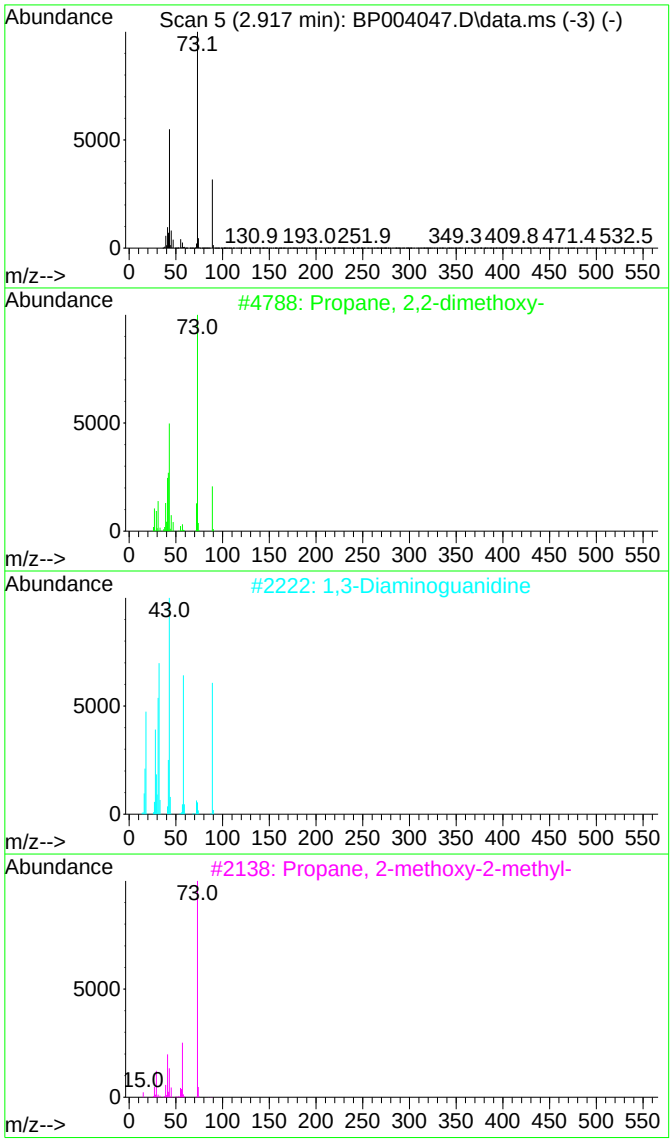
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

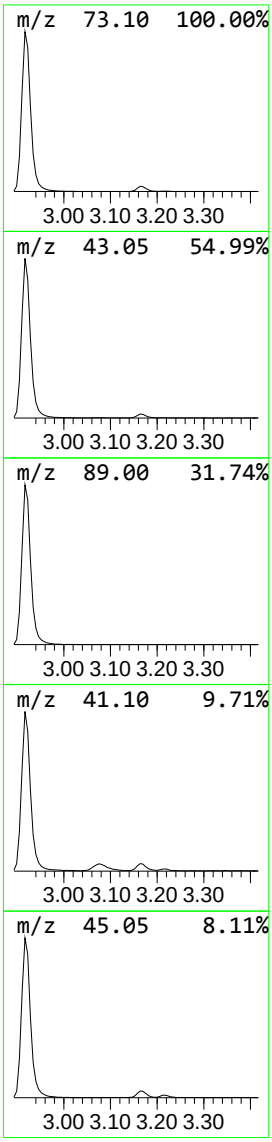
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown2.917 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.917	178.84 ng	5938360	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Data File : BP004047.D
Acq On : 21 Nov 2020 20:21
Operator : CG/JU
Sample : L4839-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B5-7-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
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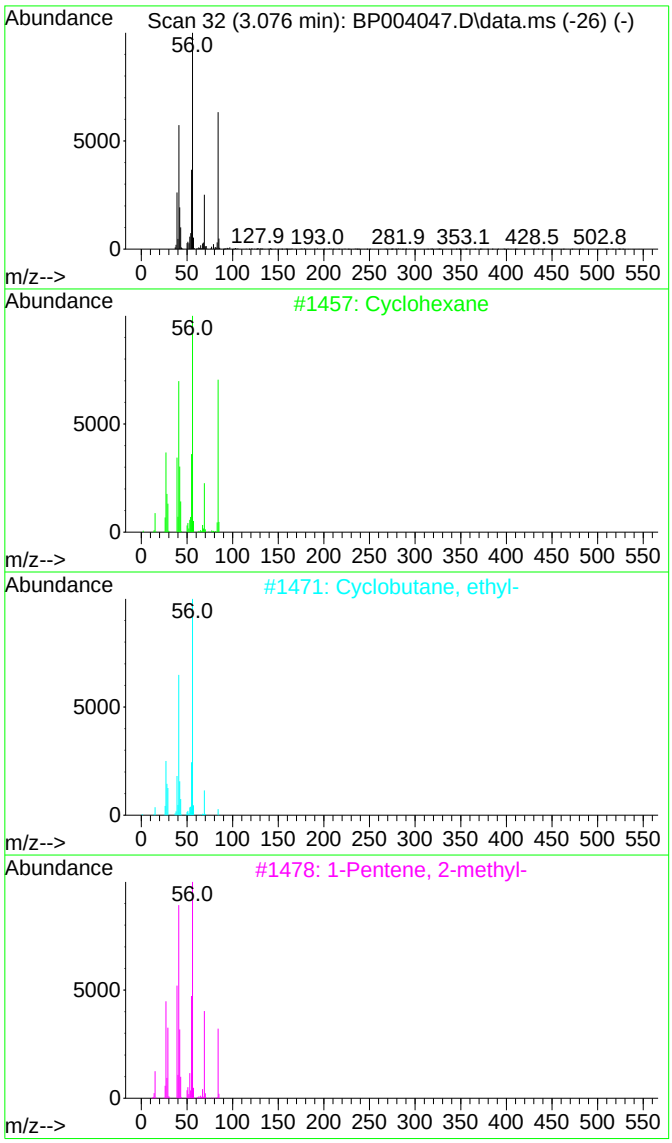
TIC Integration Parameters: LSCINT.P

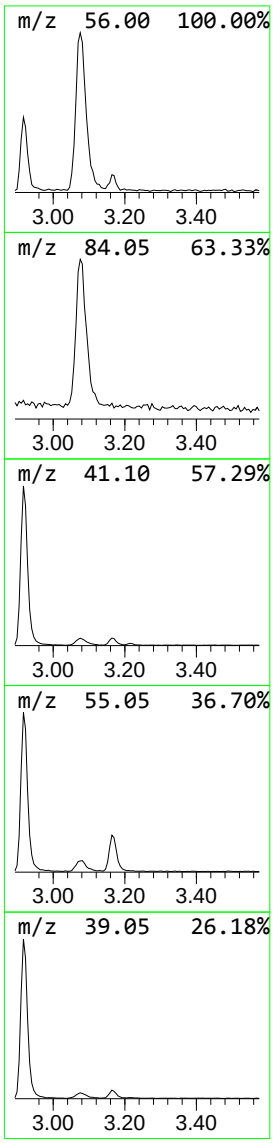
****

Peak Number 2 Cyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.076	3.58 ng	119001	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
4	1-Hexene	84	C6H12	000592-41-6	56
5	1-Octene, 2-methyl-	126	C9H18	004588-18-5	50





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Sample : L4839-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B5-7-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
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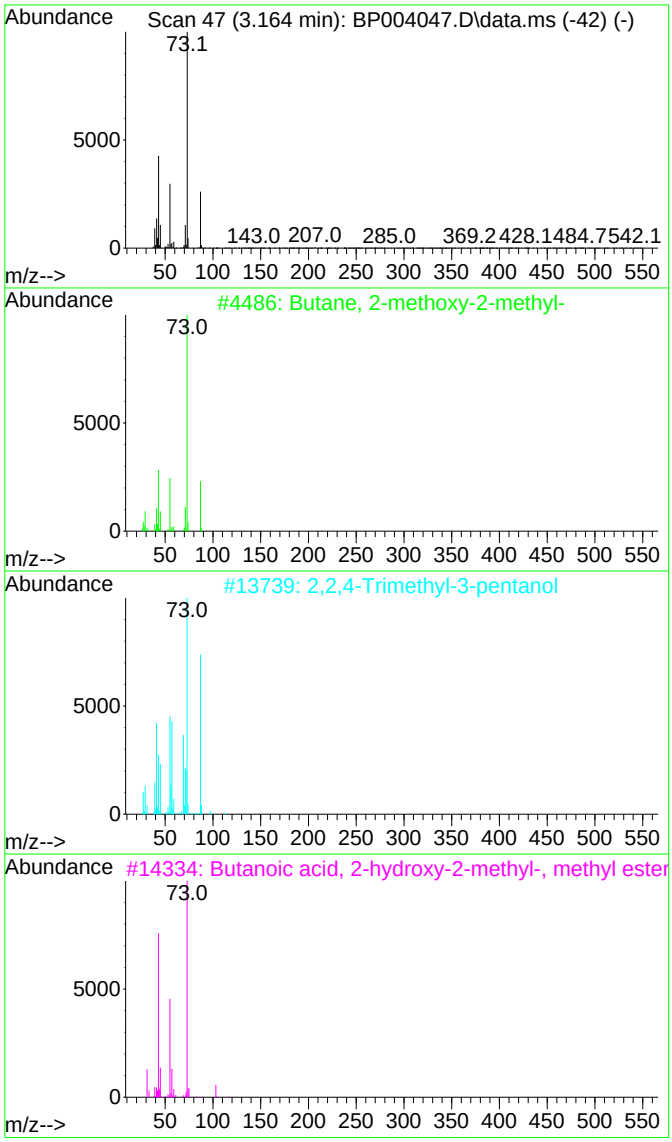
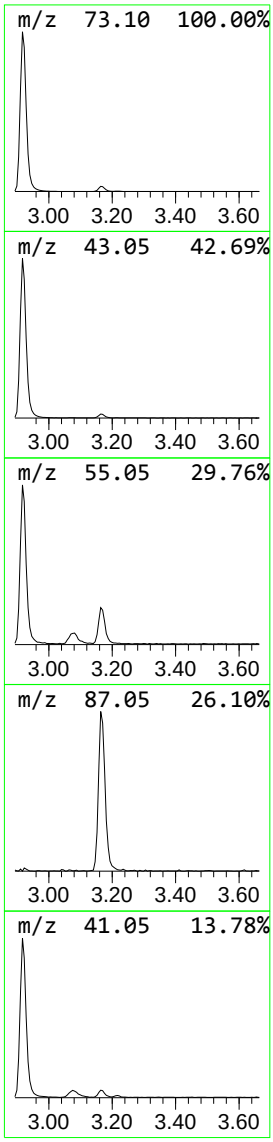
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.164	7.18 ng	238455	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Sample : L4839-02
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B5-7-8

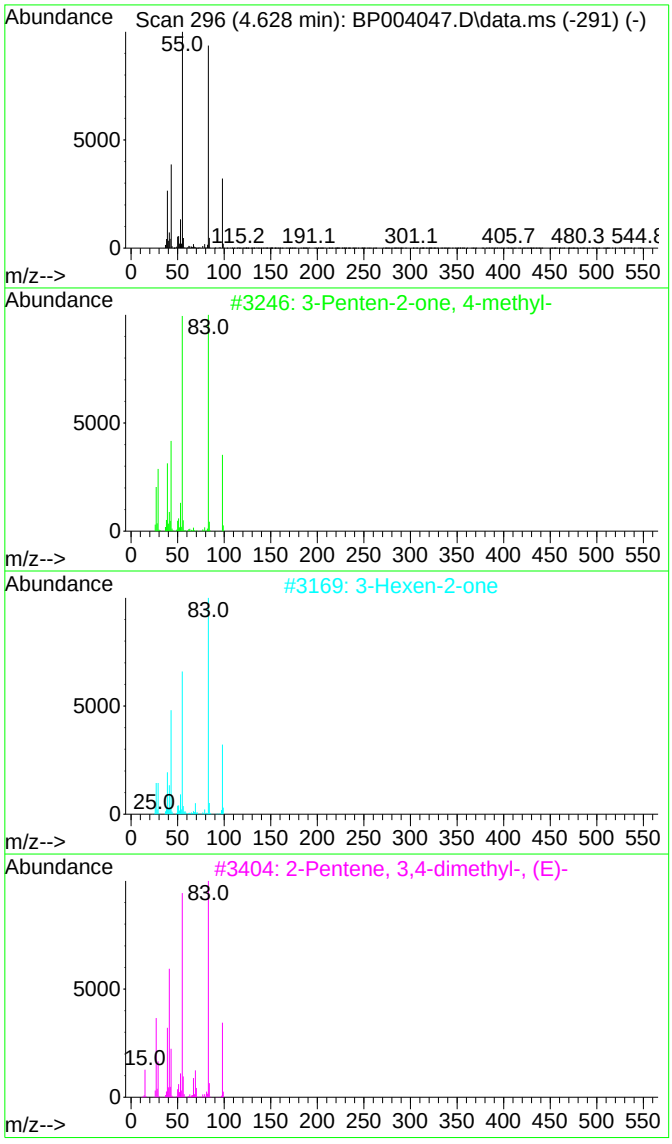
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

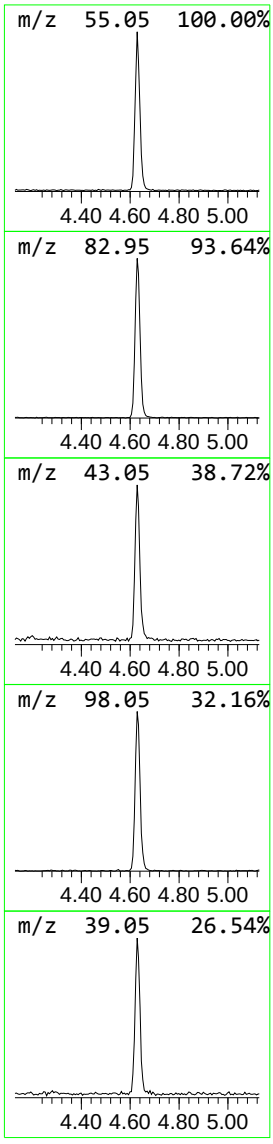
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.628	6.64 ng	220652	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Sample : L4839-02
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B5-7-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
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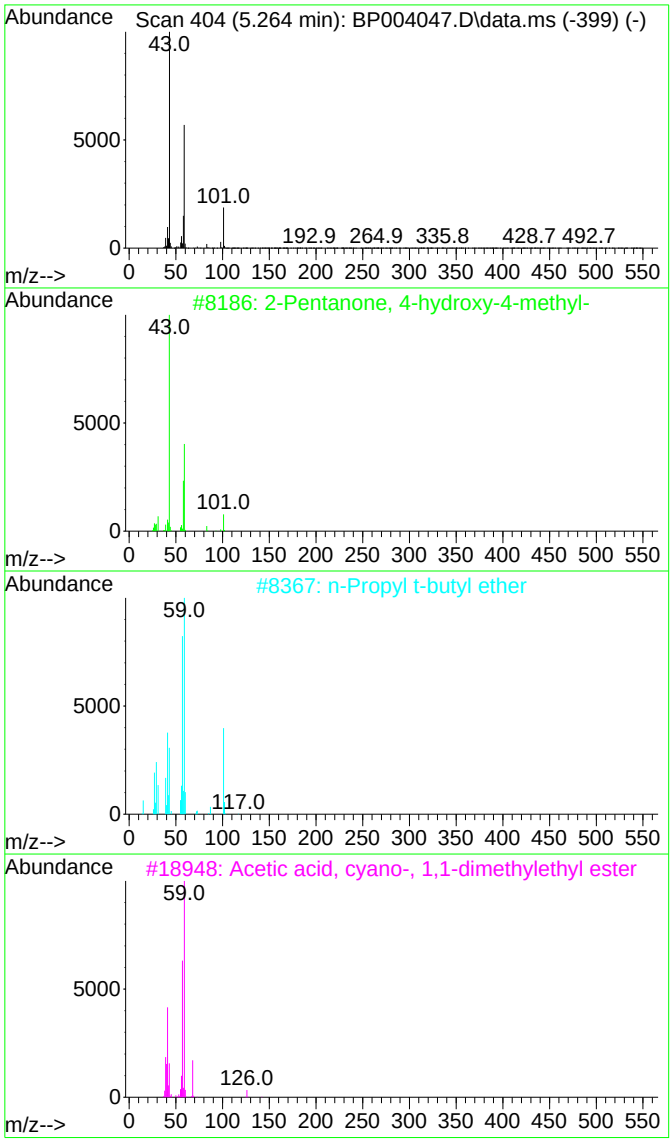
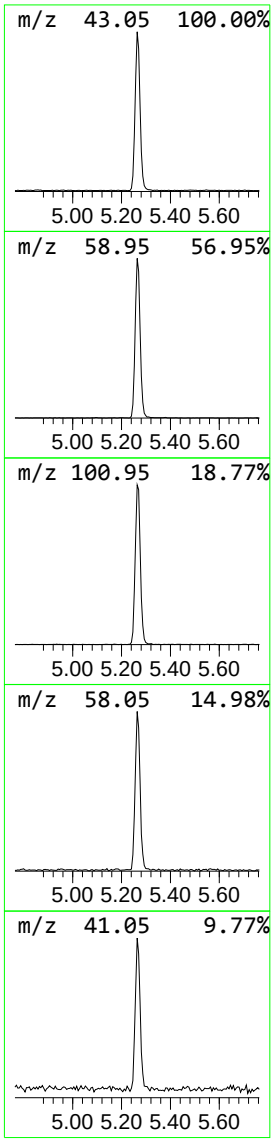
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.264	6.94 ng	230328	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





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BNA_P
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
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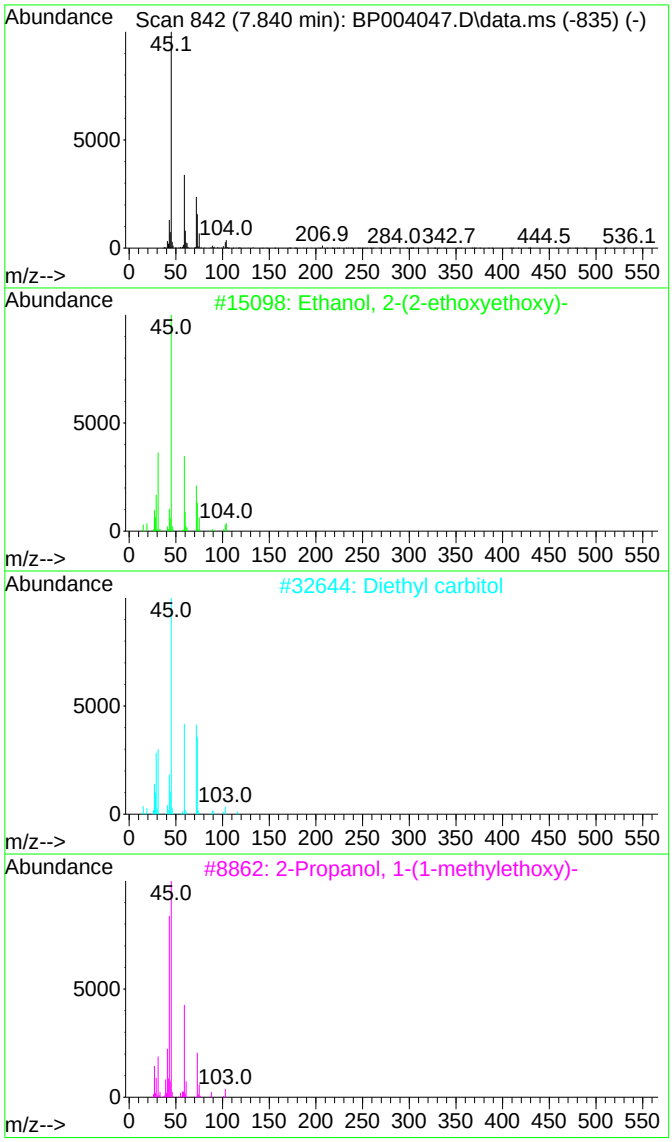
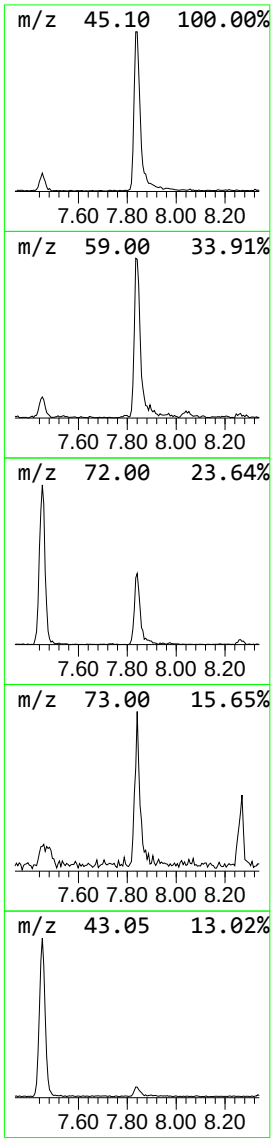
****
Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.840	2.14 ng	71167	1,4-Dichlorobenzene-d4	8.263

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	78
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39





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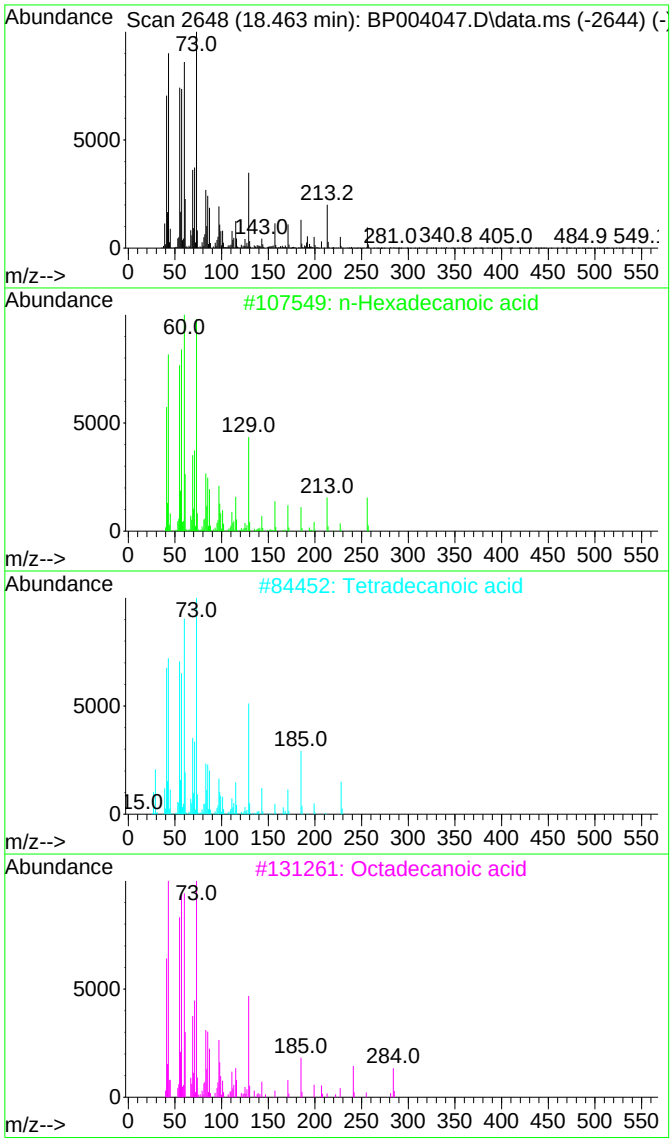
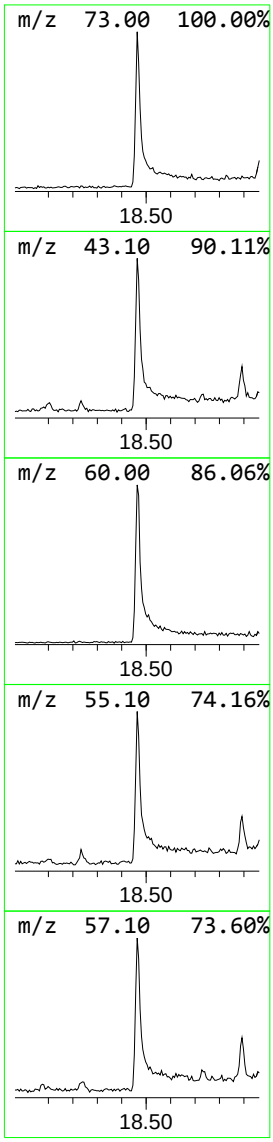
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.463	6.87 ng	441609	Phenanthrene-d10	17.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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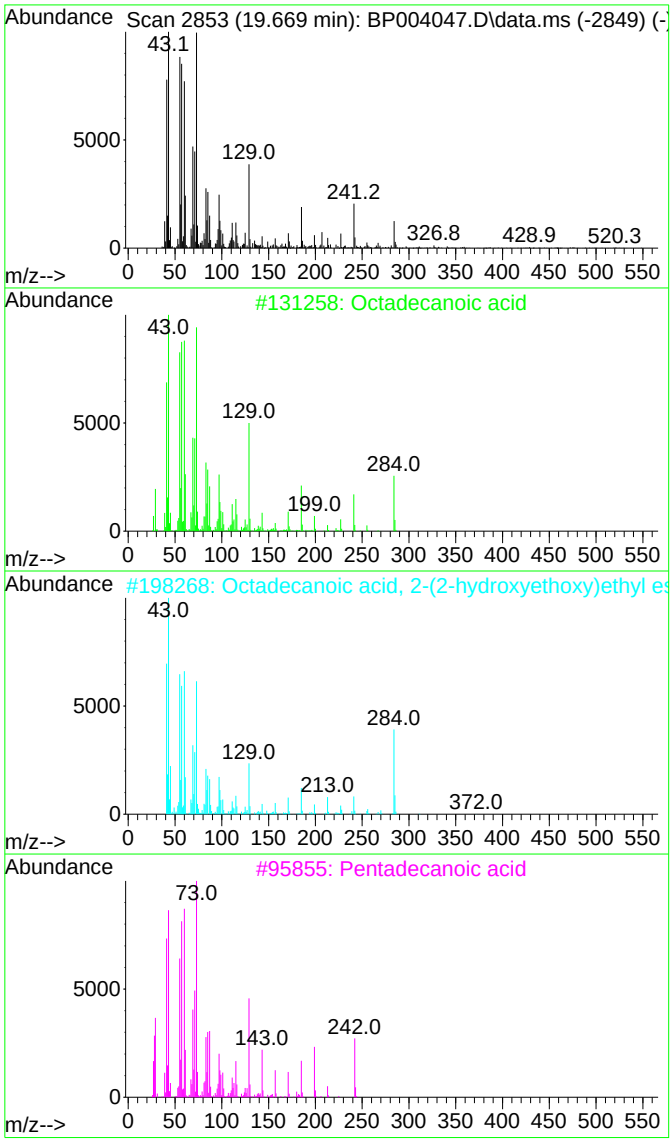
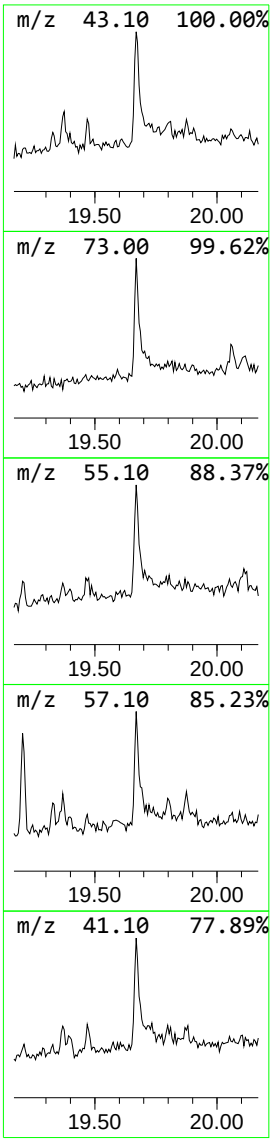
****

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.669	2.60 ng	189225	Chrysene-d12	21.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





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Operator : CG/JU
Sample : L4839-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B5-7-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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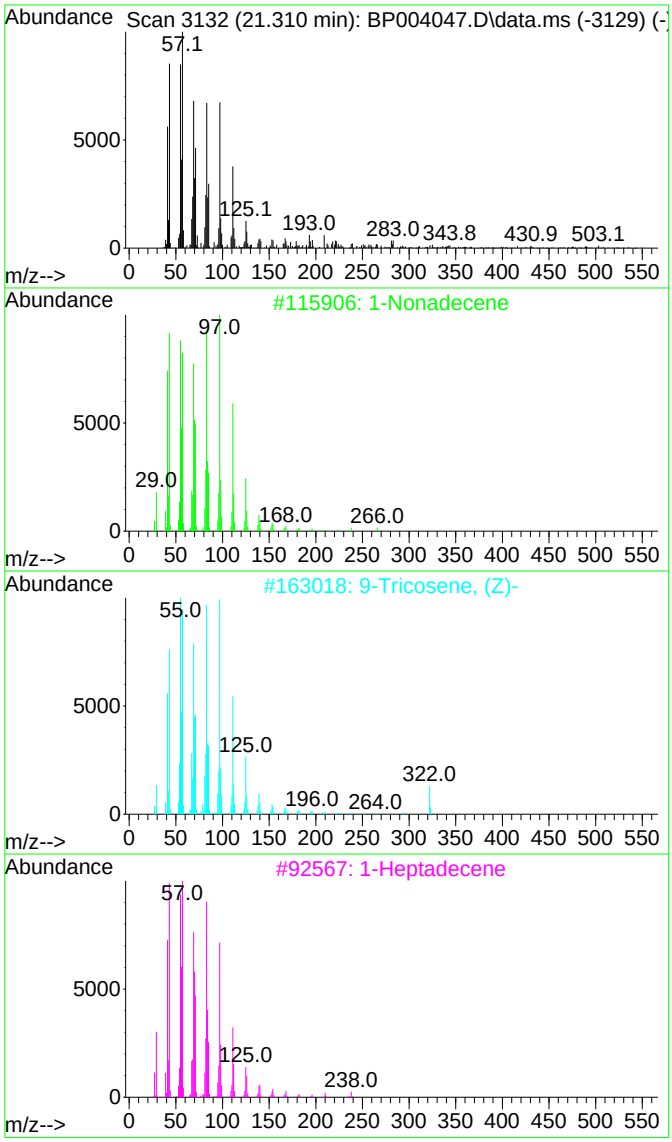
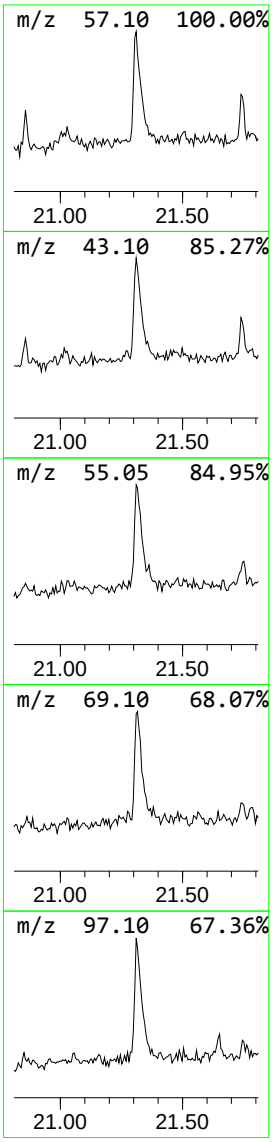
****

Peak Number 9 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.310	2.65 ng	193110	Chrysene-d12	21.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	96
3	1-Heptadecene	238	C17H34	006765-39-5	93
4	17-Pentatriacontene	491	C35H70	006971-40-0	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





Tentatively Identified Compound (LSC) summary

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Data File : BP004047.D
Acq On : 21 Nov 2020 20:21
Operator : CG/JU
Sample : L4839-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B5-7-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.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
unknown2.917	2.917	178.8	ng	5938360	1	8.263	664114	20.0
Cyclohexane	3.076	3.6	ng	119001	1	8.263	664114	20.0
Butane, 2-metho...	3.164	7.2	ng	238455	1	8.263	664114	20.0
3-Penten-2-one,...	4.628	6.6	ng	220652	1	8.263	664114	20.0
2-Pentanone, 4-...	5.264	6.9	ng	230328	1	8.263	664114	20.0
Ethanol, 2-(2-e...	7.840	2.1	ng	71167	1	8.263	664114	20.0
n-Hexadecanoic ...	18.463	6.9	ng	441609	4	17.616	1285050	20.0
Octadecanoic acid	19.669	2.6	ng	189225	5	21.651	1455180	20.0
1-Nonadecene	21.310	2.6	ng	193110	5	21.651	1455180	20.0