LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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: BM033312.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.654	49	54	63	rBV2	233408	327532	4.48%	0.903%
2	4.354	168	173	180	rBV	110730	166575	2.28%	0.459%
3	4.419	180	184	186	rVV2	81686	107806	1.47%	0.297%
4	4.449	186	189	194	rVB	97410	130803	1.79%	0.361%
5	5.043	285	290	297	rBV	149321	219567	3.00%	0.606%
6	5.513	363	370	378	rVB	1094604	1656185	22.65%	4.568%
7	6.119	468	473	479	rBV	51935	76781	1.05%	0.212%
8	7.101	632	640	651	rBV2	639248	1215703	16.63%	3.353%
9	7.325	671	678	685	rVB6	47056	109247	1.49%	0.301%
10	7.925	768	780	787	rBV	446683	737746	10.09%	2.035%
11	8.019	791	796	799	rVV2	47879	88392	1.21%	0.244%
12	8.072	799	805	813	rVV	106669	237510	3.25%	0.655%
13	8.195	813	826	837	rVV2	294458	697754	9.54%	1.924%
14	8.295	837	843	851	rVB	153768	260892	3.57%	0.720%
15	8.578	883	891	895	rBV5	38876	73547	1.01%	0.203%
16	8.919	929	949	954	rBV3	202044	727960	9.96%	2.008%
17	8.989	954	961	965	rBV	345006	682633	9.34%	1.883%
18	9.089	971	978	985	rVB	1638875	2864283	39.18%	7.899%
19	9.354	1018	1023	1033	rVB8	32811	75124	1.03%	0.207%
20	9.719	1081	1085	1097	rVB	133211	265078	3.63%	0.731%
21	10.495	1211	1217	1224	rBV	210137	348325	4.76%	0.961%
22	10.719	1247	1255	1261	rBV	543315	962792	13.17%	2.655%
23	11.330	1350	1359	1365	rVB8	40991	99105	1.36%	0.273%
24	12.354	1525	1533	1538	rBV	62479	136788	1.87%	0.377%
25	12.589	1564	1573	1578	rBV4	72292	196771	2.69%	0.543%
26	13.171	1662	1672	1680	rBV	3630456	5325774	72.85%	14.688%
27	13.436	1713	1717	1722	rVB	74159	108809	1.49%	0.300%
28	13.554	1733	1737	1748	rVB	70876	126067	1.72%	0.348%
29	14.166	1836	1841	1848	rVB9	36863	77018	1.05%	0.212%
30	14.348	1866	1872	1879	rBV4	37840	91908	1.26%	0.253%
31	14.548	1900	1906	1914	rBV	780377	1166191	15.95%	3.216%
32	16.036	2152	2159	2174	rBV	2616573	4041385	55.28%	11.146%
33	17.289	2366	2372	2379	rBV	893162	1399486	19.14%	3.860%
34	17.942	2480	2483	2488	rVB2	67311	87823	1.20%	0.242%
35	18.165	2517	2521	2531	rBV2	111628	208204	2.85%	0.574%
36	19.112	2678	2682	2686	rBV	195332	209409	2.86%	0.578%

LSC Area Percent Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
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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

37	19.442	2734	2738	2744	rBV4	69988	122921	1.68%	0.339%
38	19.895	2810	2815	2822	rBV	5765805	7310806	100.00%	20.162%
39	21.142	3025	3027	3033	rBV2	84934	103464	1.42%	0.285%
40	21.447	3074	3079	3087	rBV	1312461	1655487	22.64%	4.566%
41	23.777	3469	3475	3485	rVB2	895059	1759797	24.07%	4.853%

Sum of corrected areas: 36259448

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
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Instrument :
BNA_M
ClientSampleId :
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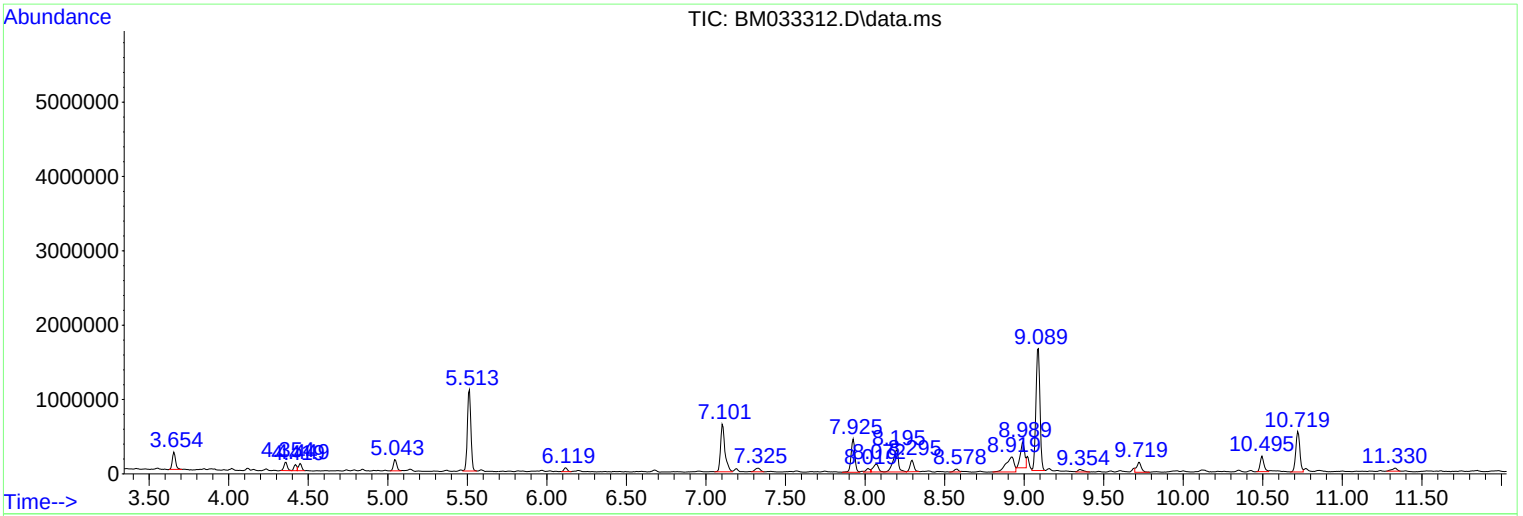
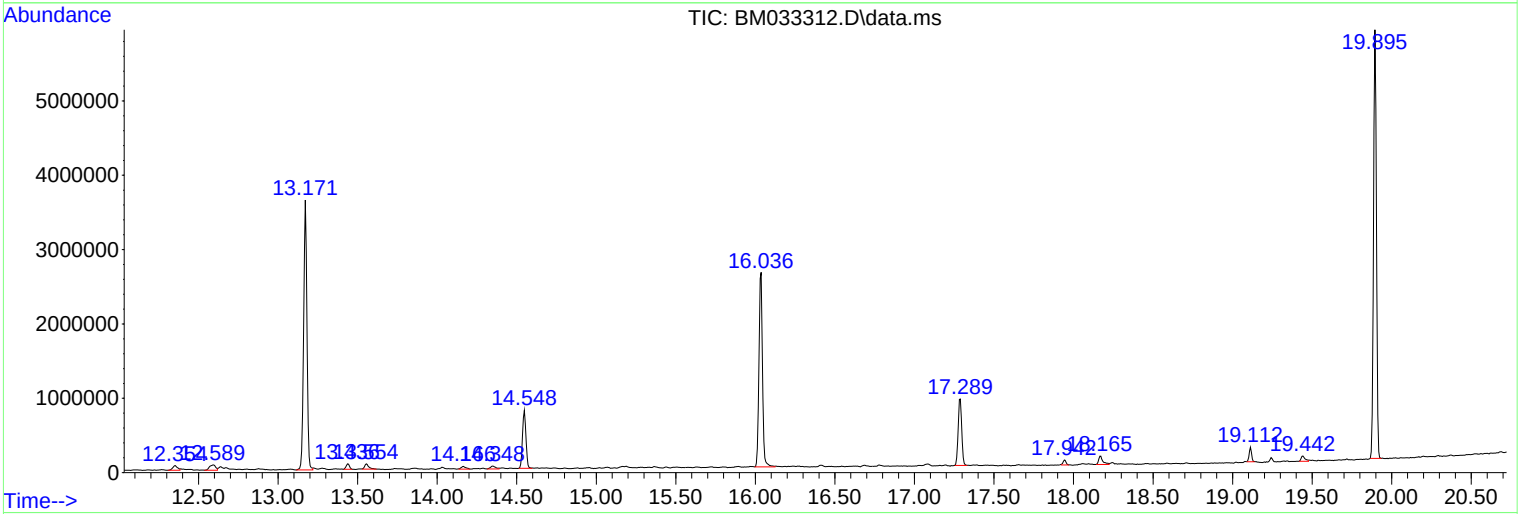
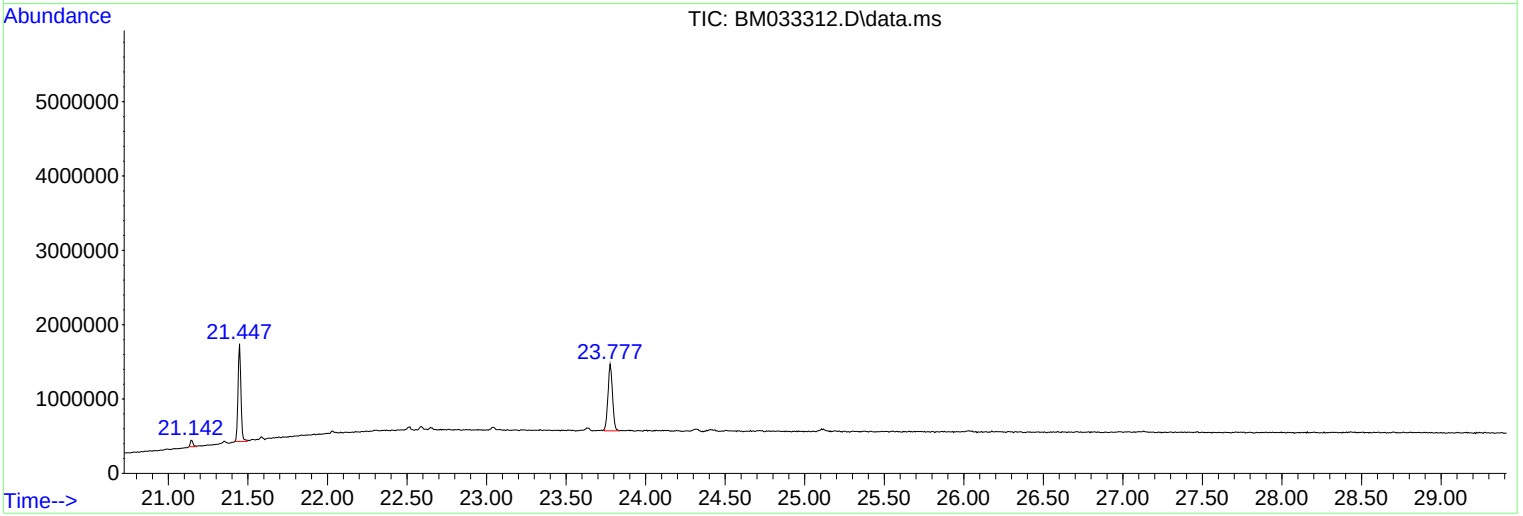
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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

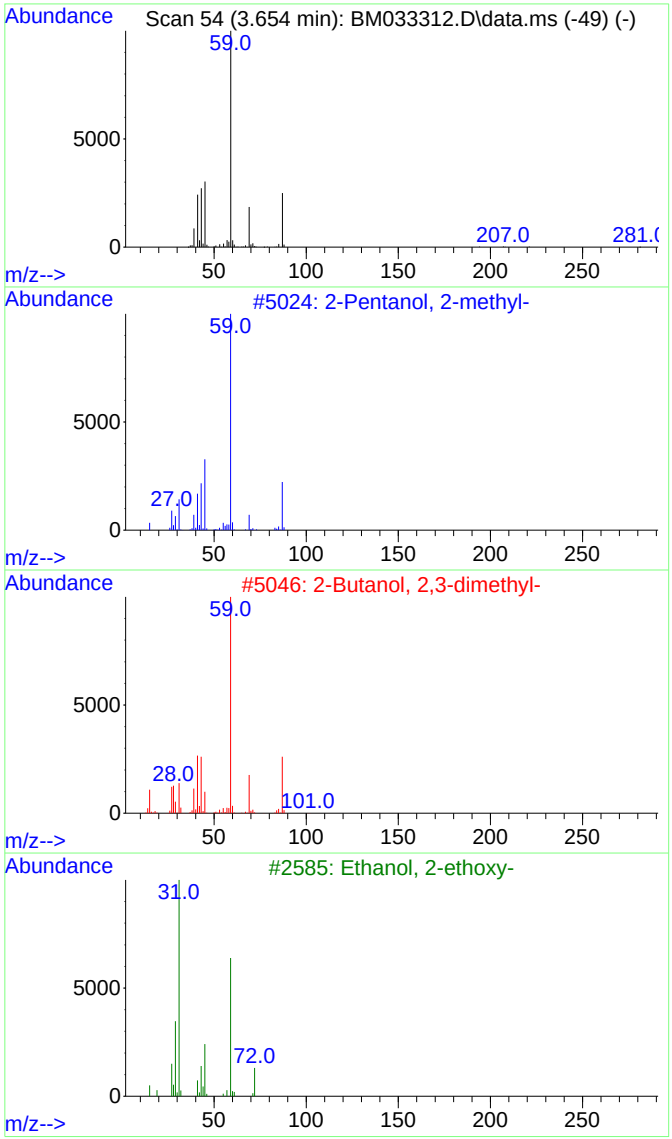
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

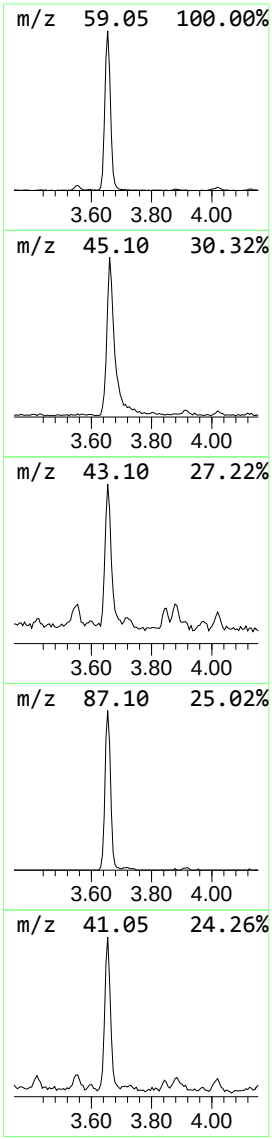
****

Peak Number 1 2-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.654	8.88 ng	327532	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72
3	Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	53
4	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	43
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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

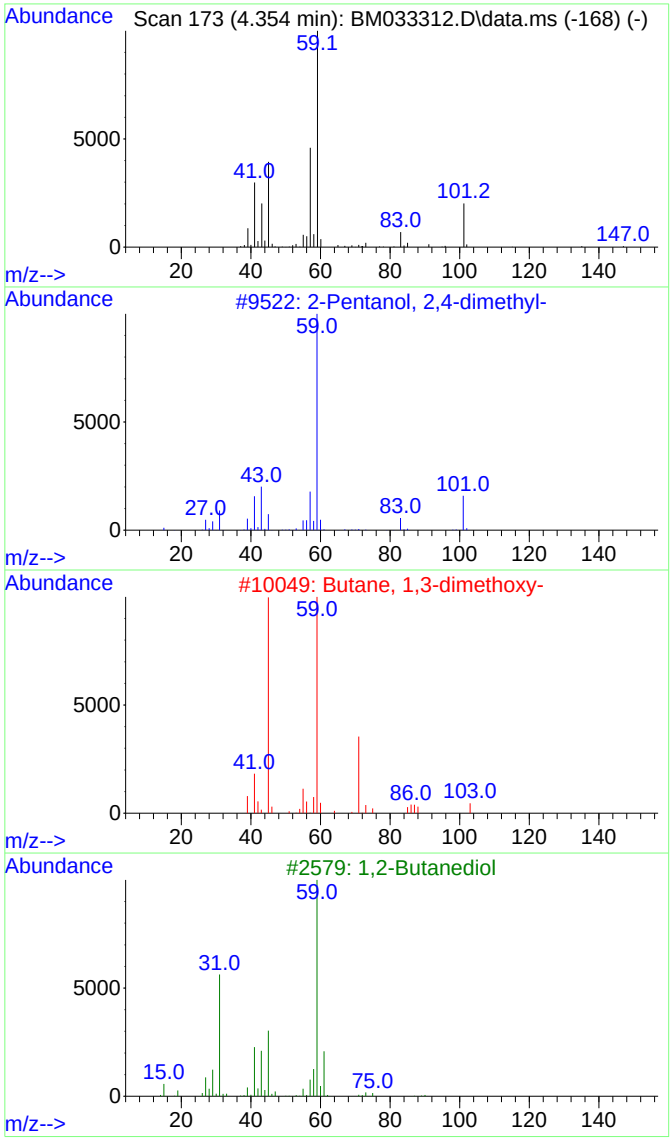
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

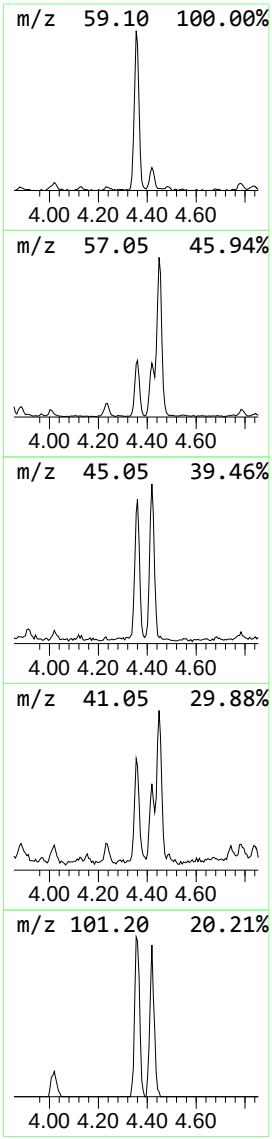
****

Peak Number 2 2-Pentanol, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.354	4.52 ng	166575	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	53
2	Butane, 1,3-dimethoxy-	118	C6H14O2	010143-66-5	45
3	1,2-Butanediol	90	C4H10O2	000584-03-2	45
4	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	43
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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

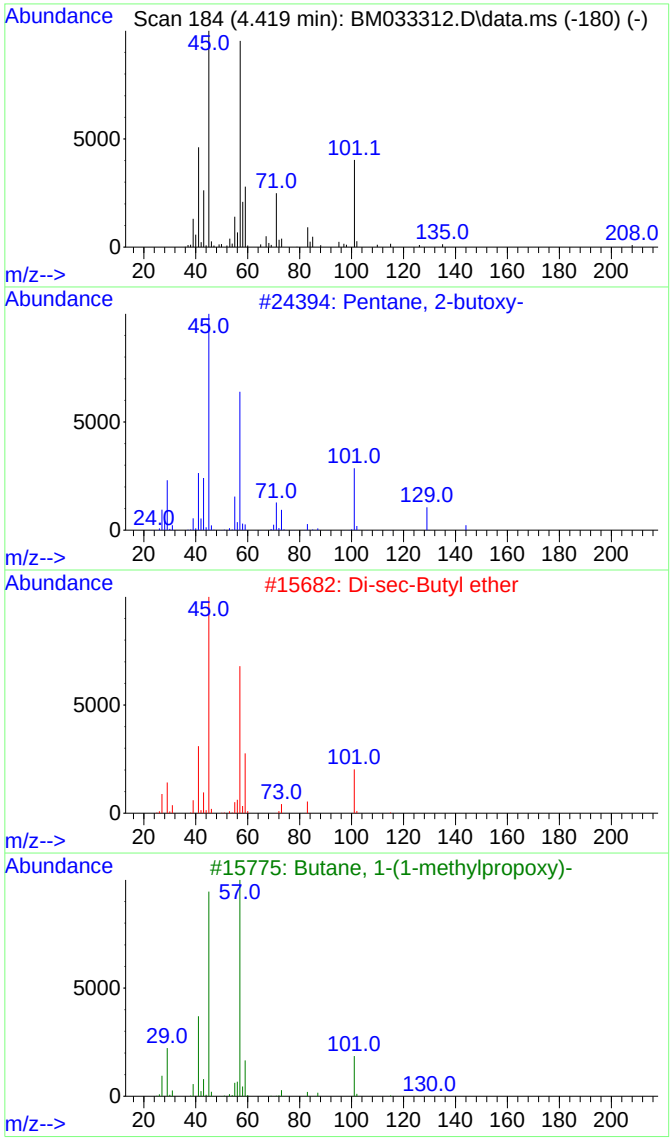
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

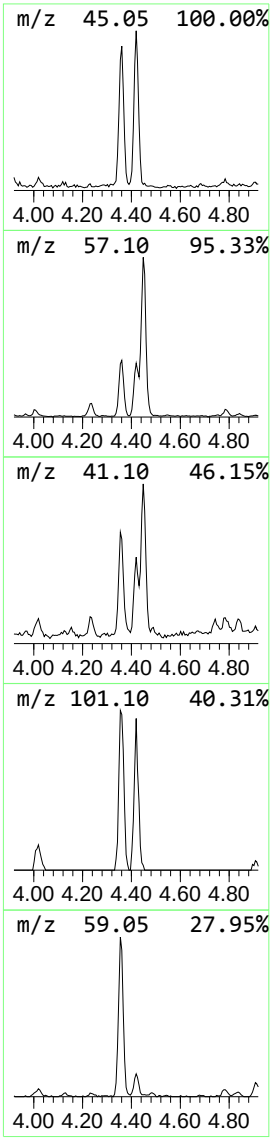
****

Peak Number 3 Pentane, 2-butoxy- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.419	2.92 ng	107806	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-butoxy-	144	C9H20O	062238-02-2	59
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42
4	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	42
5	Butane, 1,2,3,4-tetramethoxy-	178	C8H18O4	003011-85-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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

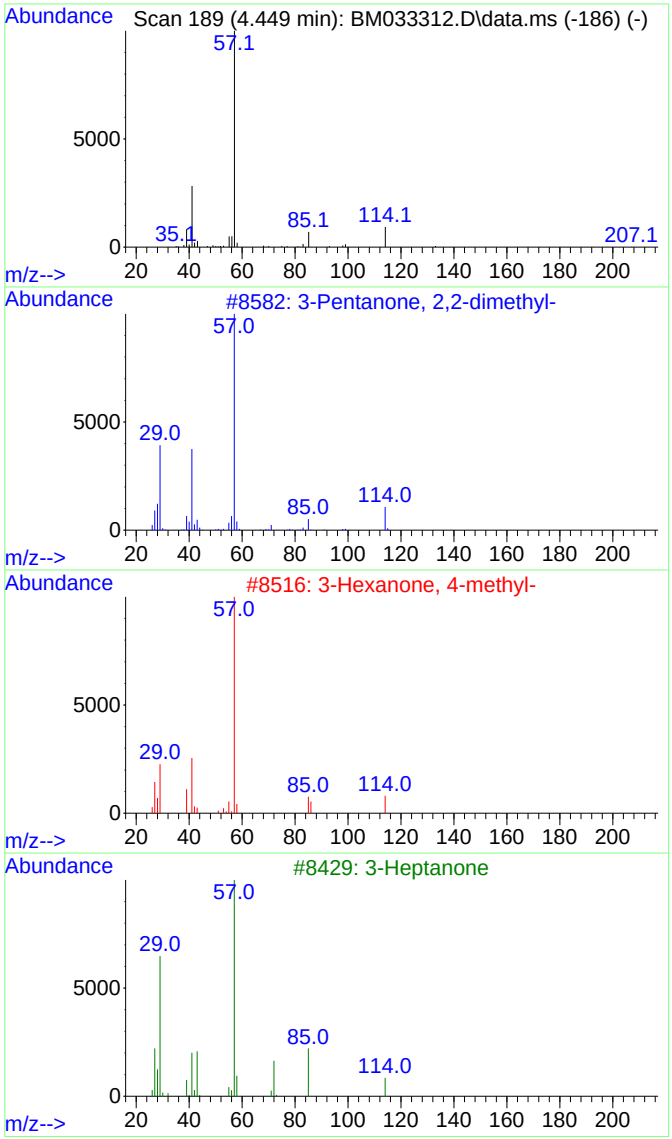
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

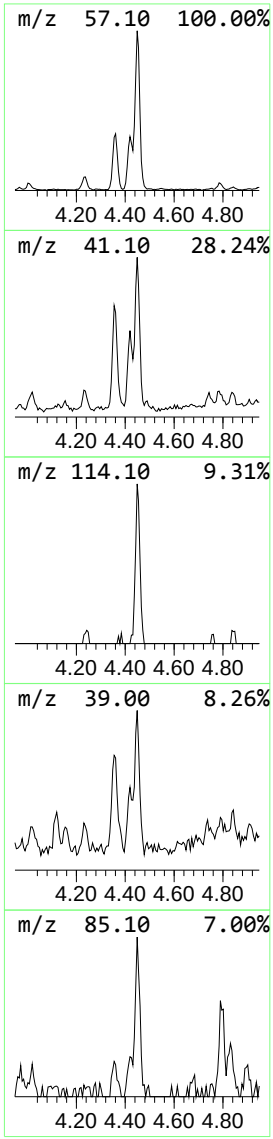
****

Peak Number 4 3-Pentanone, 2,2-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.449	3.55 ng	130803	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	59
2	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	53
3	3-Heptanone	114	C7H14O	000106-35-4	42
4	Acetic acid, [(1,1-dimethylethyl...	148	C6H12O2S	024310-22-3	25
5	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

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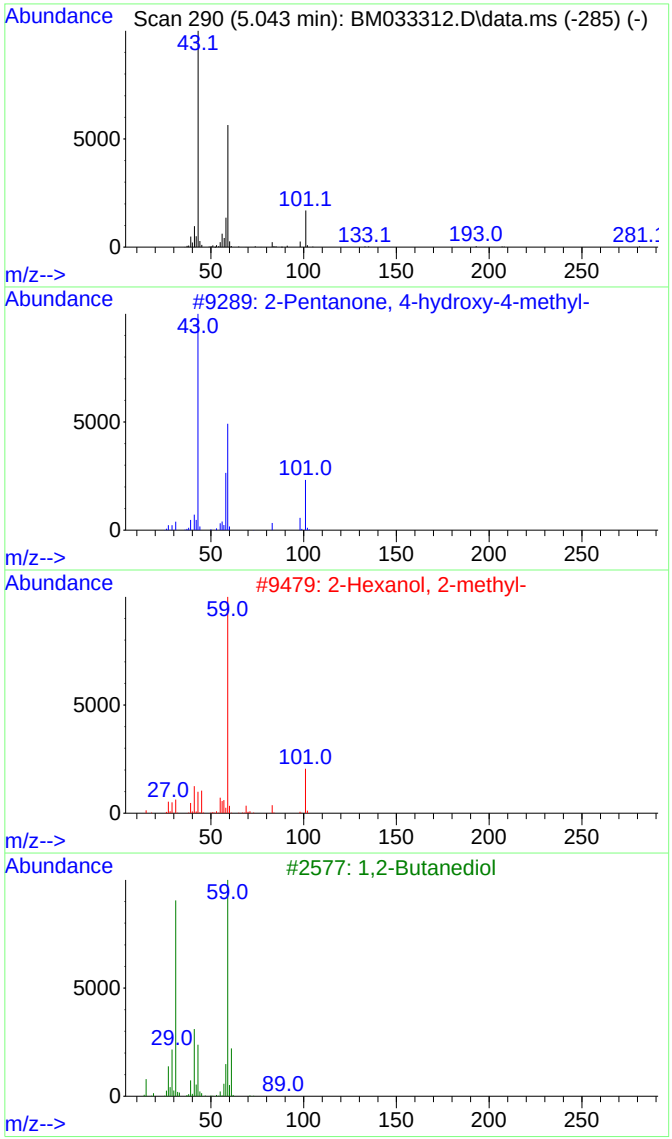
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

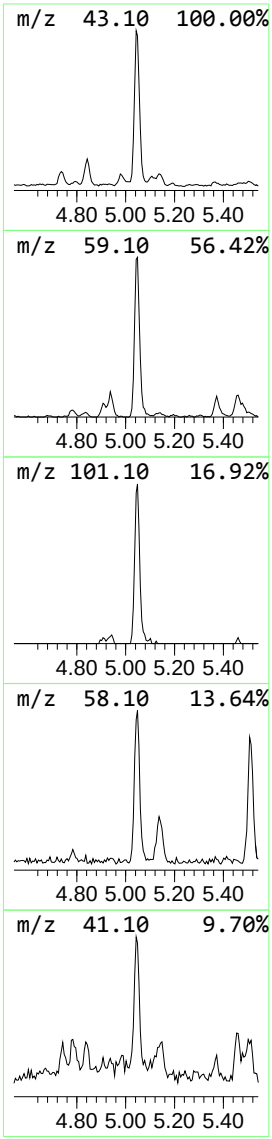
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.043	5.95 ng	219567	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	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	47
3	1,2-Butanediol	90	C4H10O2	000584-03-2	38
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	3-Octanol	130	C8H18O	000589-98-0	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
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Operator : CG/JU
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

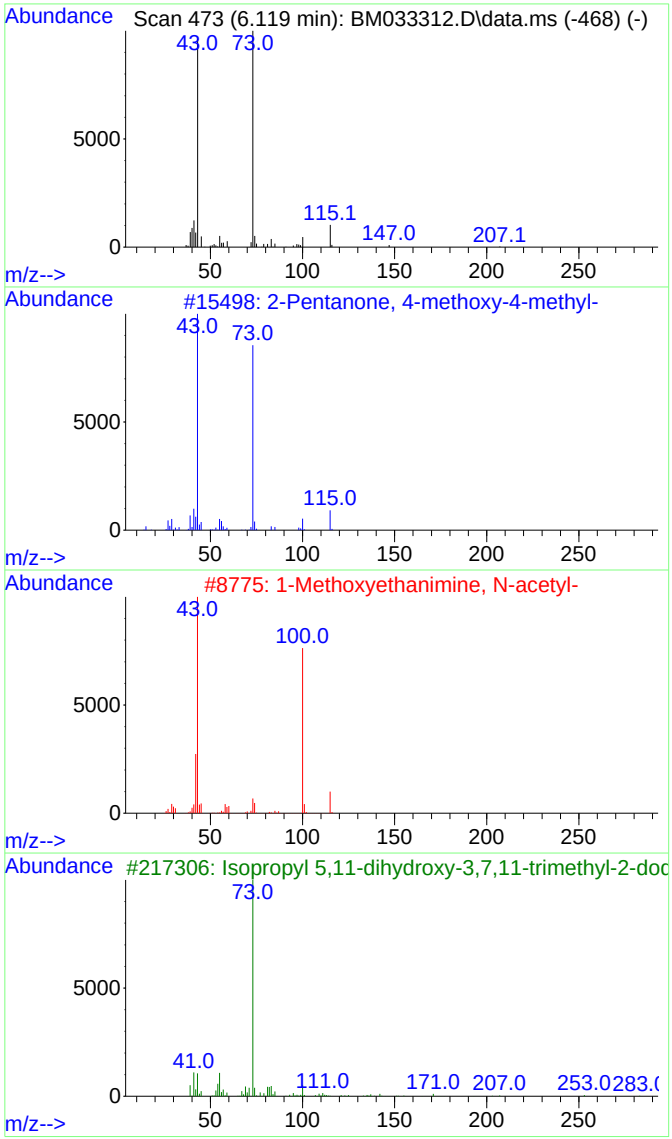
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

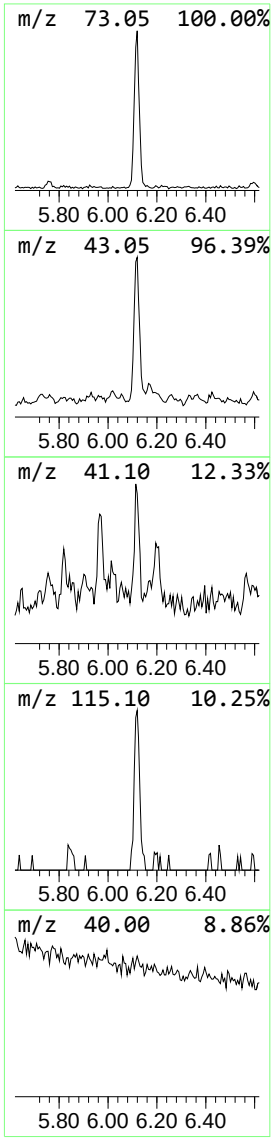
****

Peak Number 6 unknown6.119 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.119	2.08 ng	76781	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	72
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
3	Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	1000223-34-1	23
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	16
5	2-Methyl-2,4-dimethoxybutane	132	C7H16O2	039836-89-0	12





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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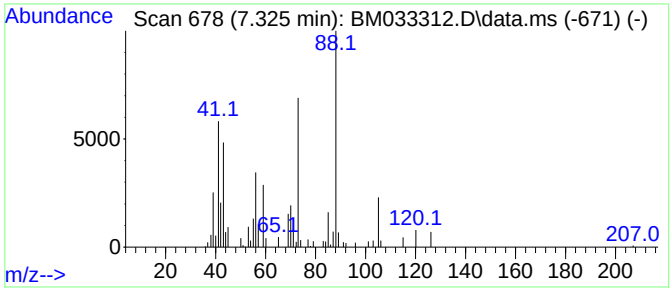
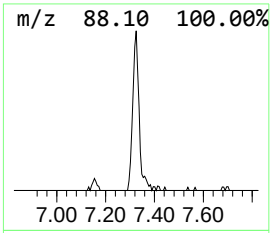
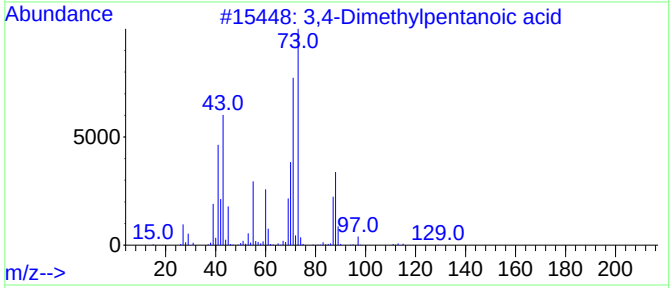
Peak Number 7 unknown7.325 Concentration Rank 15

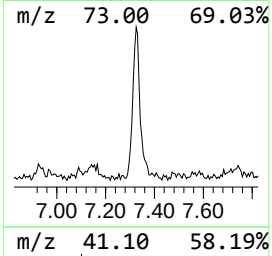
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.325	2.96 ng	109247	1,4-Dichlorobenzene-d4	7.925

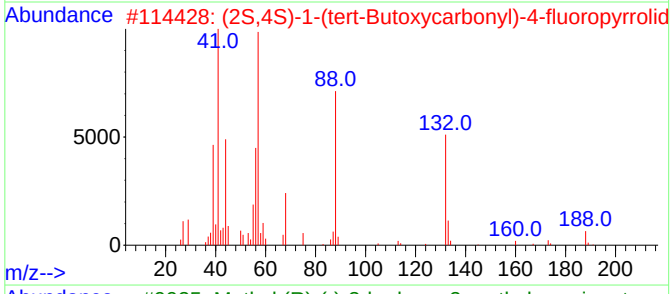
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylpentanoic acid	130	C7H14O2	003302-06-5	43
2	(2S,4S)-1-(tert-Butoxycarbonyl)-...	233	C10H16FNO4	203866-13-1	38
3	Methyl (R)-(-)-3-hydroxy-2-methy...	118	C5H10O3	072657-23-9	37
4	Aspartic acid	133	C4H7NO4	000056-84-8	35
5	Hydroxypivalic acid	118	C5H10O3	004835-90-9	32

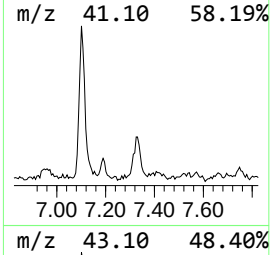


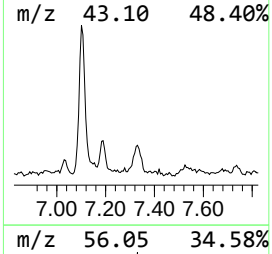


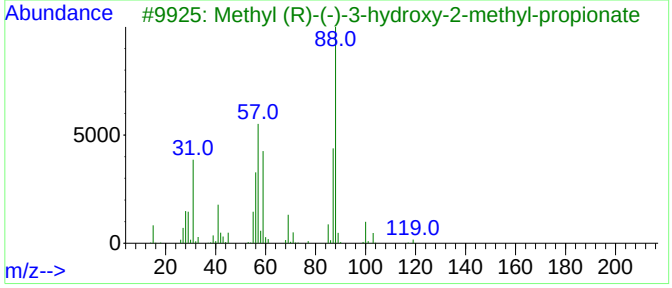


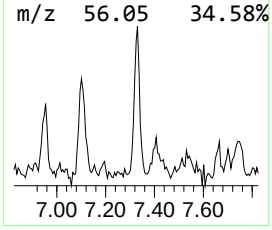












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Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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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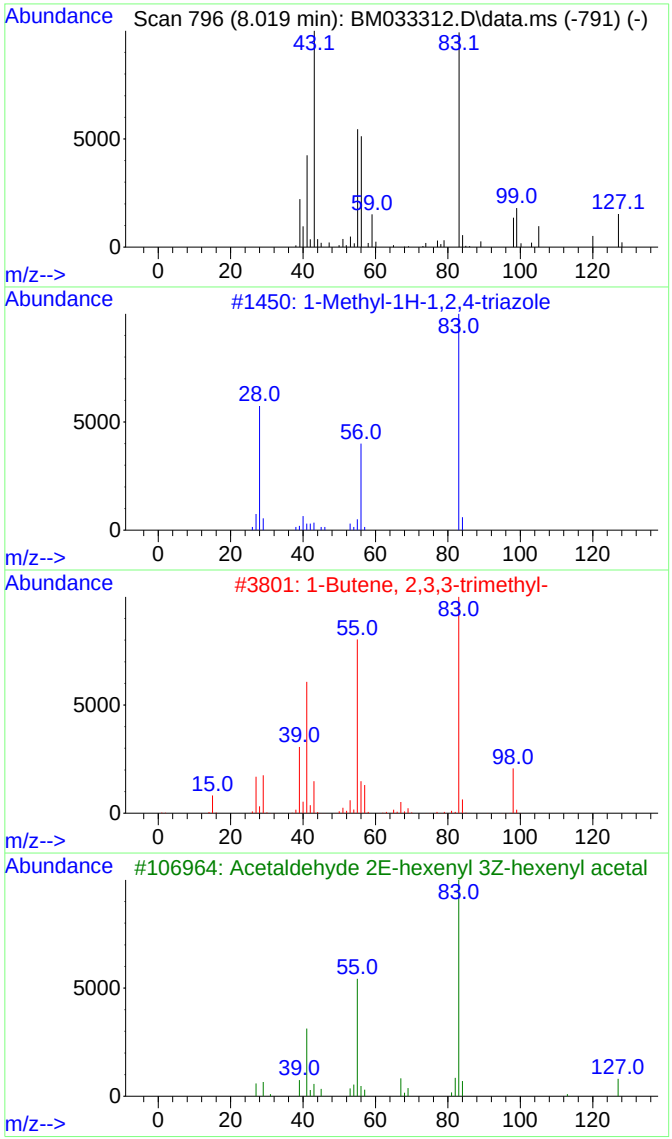
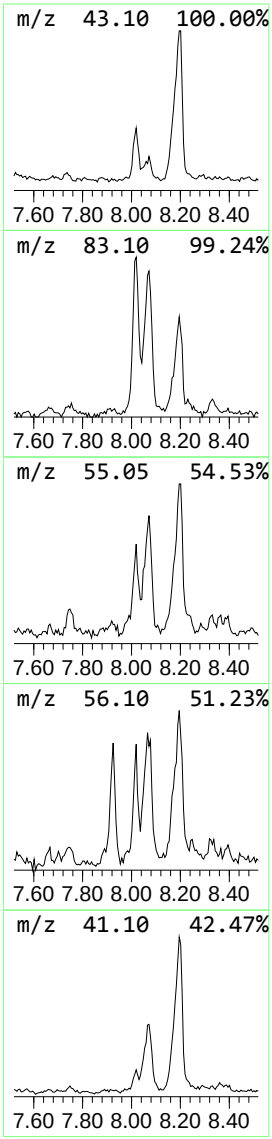
Peak Number 8 1-Methyl-1H-1,2,4-triazole Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.019	2.40 ng	88392	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	50
2	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	49
3	Acetaldehyde 2E-hexenyl 3Z-hexen...	226	C14H26O2	1000431-45-5	43
4	1-Propoxypropan-2-yl 2-methylbut...	200	C11H20O3	1000367-10-6	38
5	Cyclopropane, 2-bromo-1,1,3-trim...	162	C6H11Br	036617-00-2	38





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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

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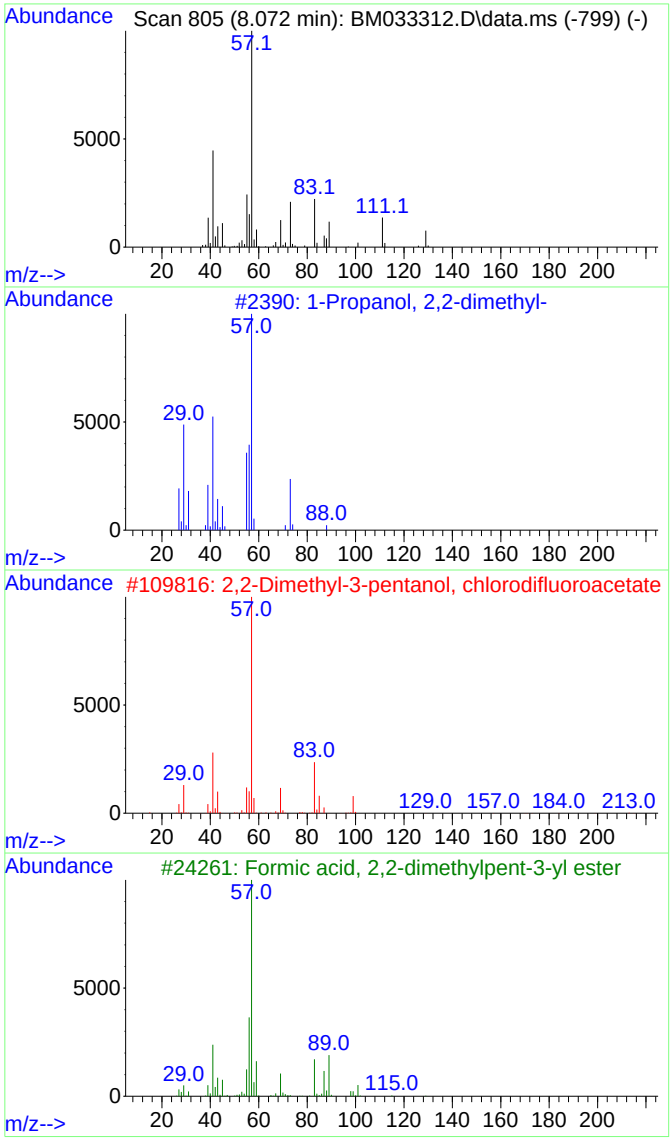
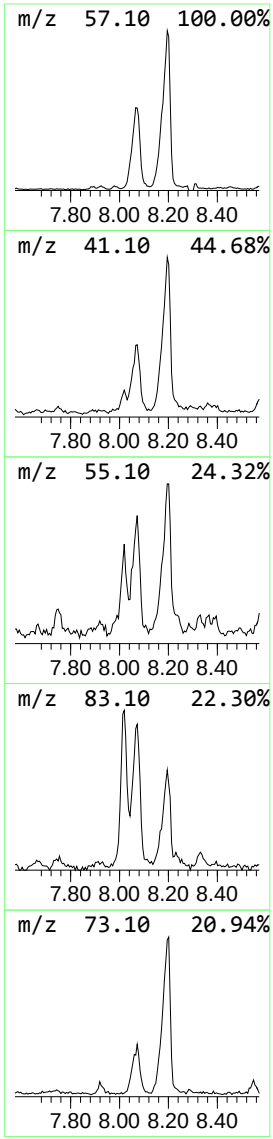
Peak Number 9 unknown8.072 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.072	6.44 ng	237510	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	27
2	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	25
3	Formic acid, 2,2-dimethylpent-3-...	144	C8H16O2	1000368-88-1	23
4	1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	16
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	14





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

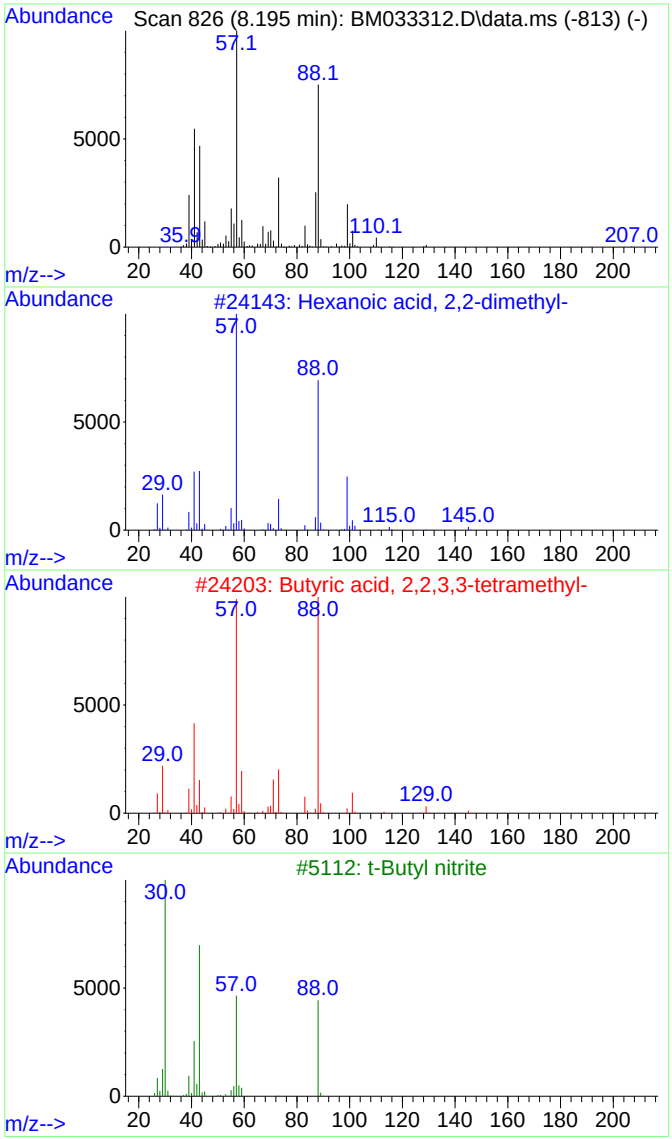
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

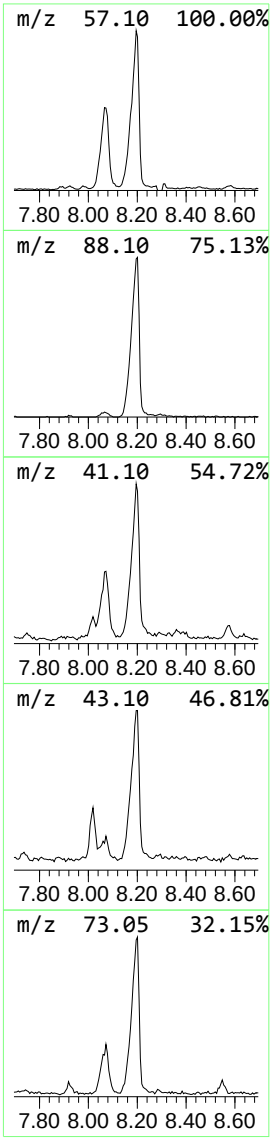
****

Peak Number 10 Hexanoic acid, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.195	18.92 ng	697754	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	59
2	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	53
3	t-Butyl nitrite	103	C4H9NO2	000540-80-7	43
4	Methyl propionate	88	C4H8O2	000554-12-1	43
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	40





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Misc :
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Instrument :
BNA_M
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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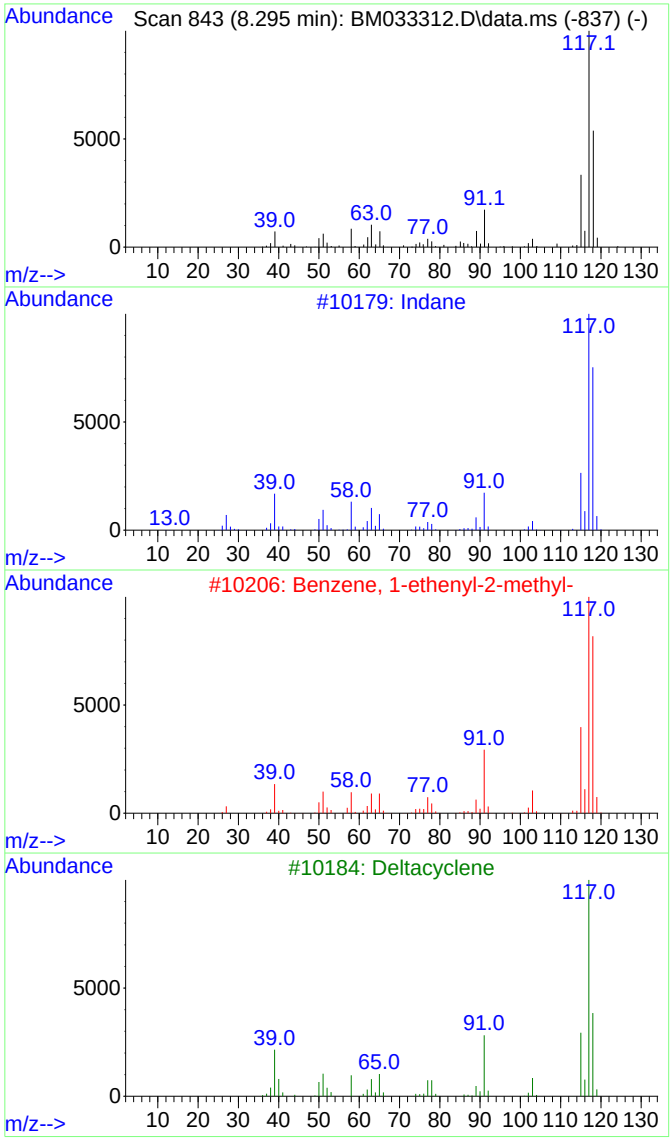
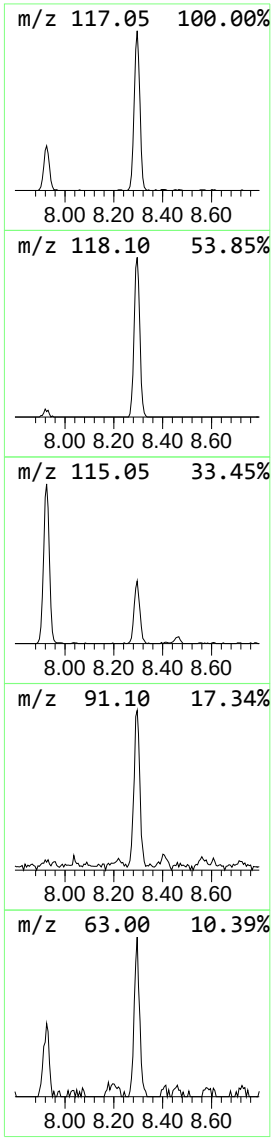
Peak Number 11 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.295	7.07 ng	260892	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
3	Deltacyclene	118	C9H10	007785-10-6	68
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	55





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Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

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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

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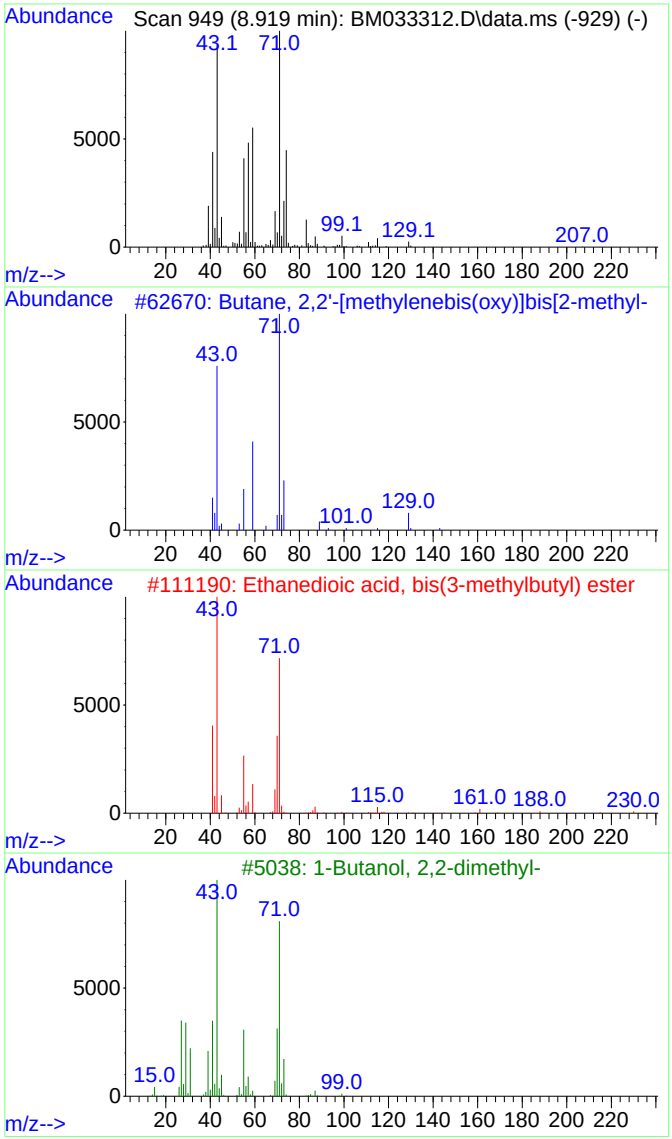
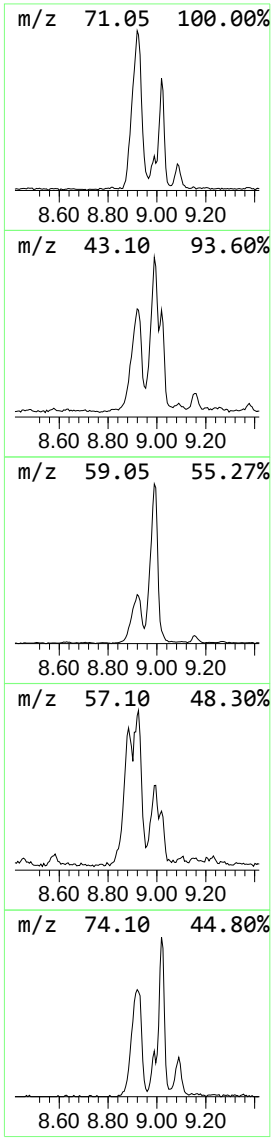
Peak Number 12 unknown8.919 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.919	19.73 ng	727960	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2'-[methylenebis(oxy)]...	188	C11H24O2	054699-28-4	43
2	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	38
3	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	37
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	27
5	Ether, 3-butenyl pentyl	142	C9H18O	034061-78-4	27





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Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

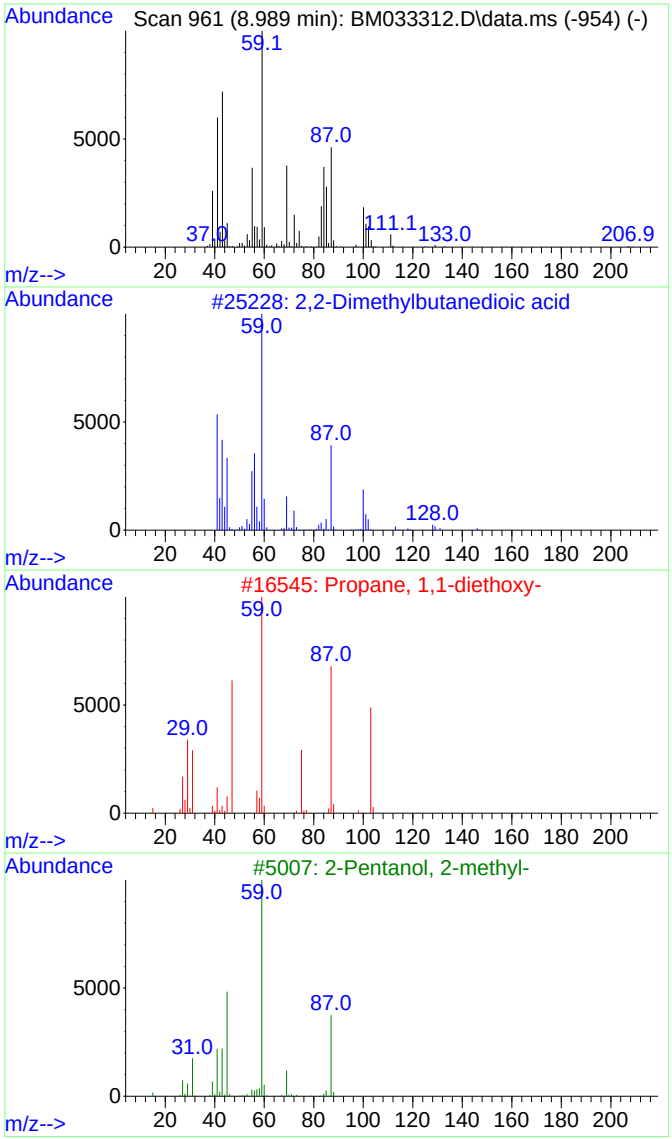
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

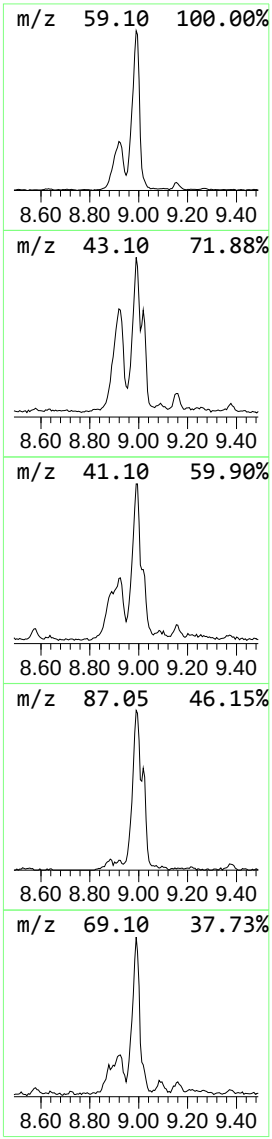
****

Peak Number 13 unknown8.989 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.989	18.51 ng	682633	1,4-Dichlorobenzene-d4	7.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylbutanedioic acid	146	C6H10O4	000597-43-3	45
2	Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	43
3	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	38
4	Allyldimethylsilane	100	C5H12Si	003937-30-2	38
5	Isopropyldimethylsilane	102	C5H14Si	1000433-69-3	38





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Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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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
TIC Integration Parameters: LSCINT.P

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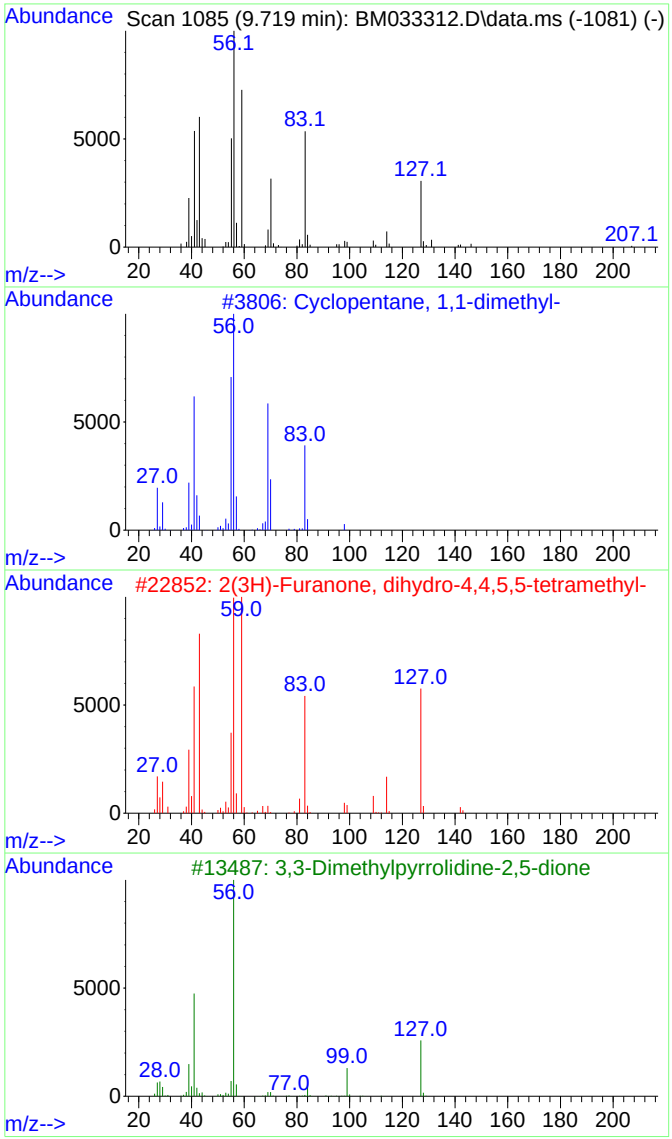
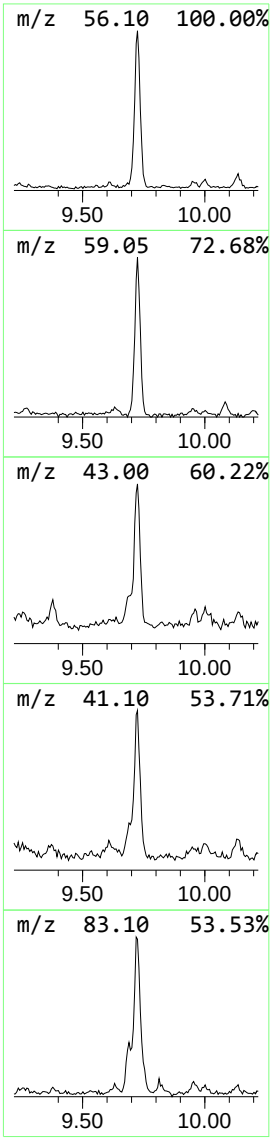
Peak Number 14 unknown9.719 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.719	5.51 ng	265078	Naphthalene-d8	10.719

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	49
2	2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	43
3	3,3-Dimethylpyrrolidine-2,5-dione	127	C6H9NO2	003437-29-4	38
4	2-Methylcyclohexylamine	113	C7H15N	007003-32-9	38
5	2(3H)-Furanone, dihydro-3,3-dime...	114	C6H10O2	003709-08-8	38





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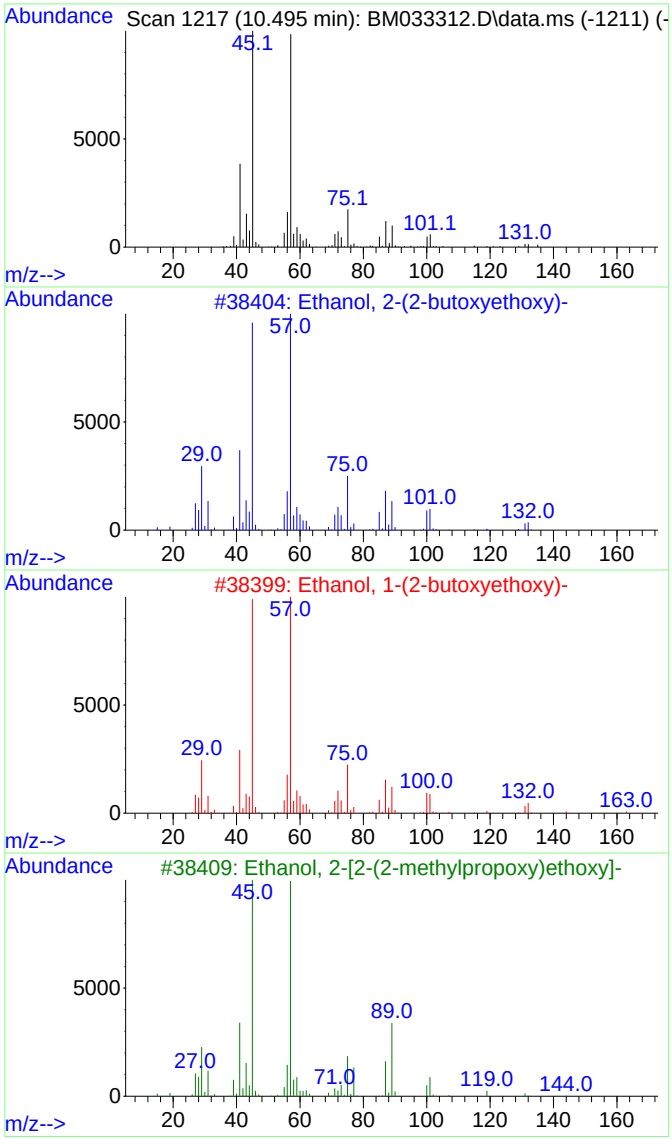
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

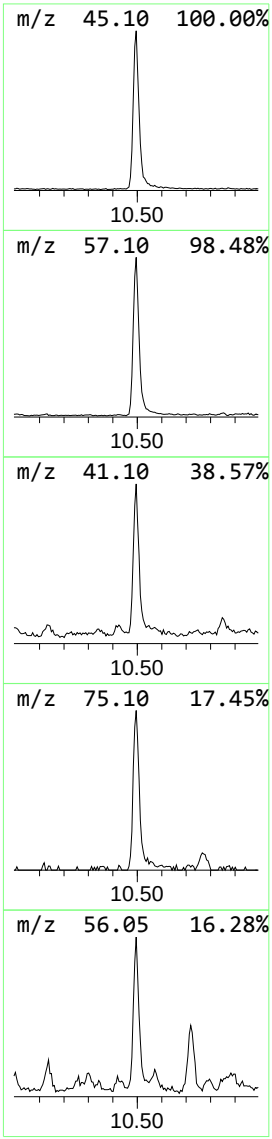
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.495	7.24 ng	348325	Naphthalene-d8	10.719

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	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50





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ALS Vial : 9 Sample Multiplier: 1

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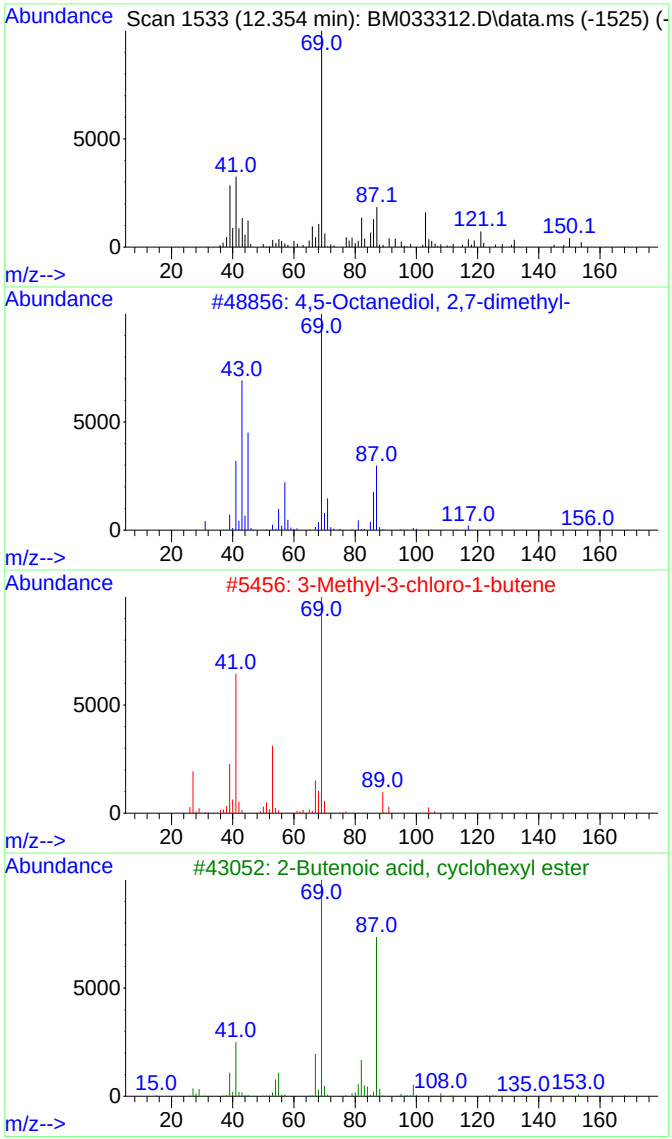
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

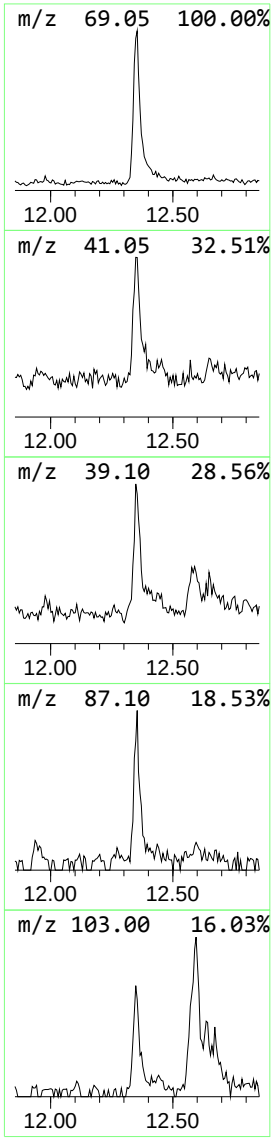
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 4,5-Octanediol, 2,7-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.354	2.84 ng	136788	Naphthalene-d8	10.719

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-Octanediol, 2,7-dimethyl-	174	C10H22O2	1000153-20-8	50
2	3-Methyl-3-chloro-1-butene	104	C5H9Cl	002190-48-9	47
3	2-Butenoic acid, cyclohexyl ester	168	C10H16O2	016491-62-6	47
4	1-Octen-4-ol	128	C8H16O	040575-42-6	47
5	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	46





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ClientSampleId :
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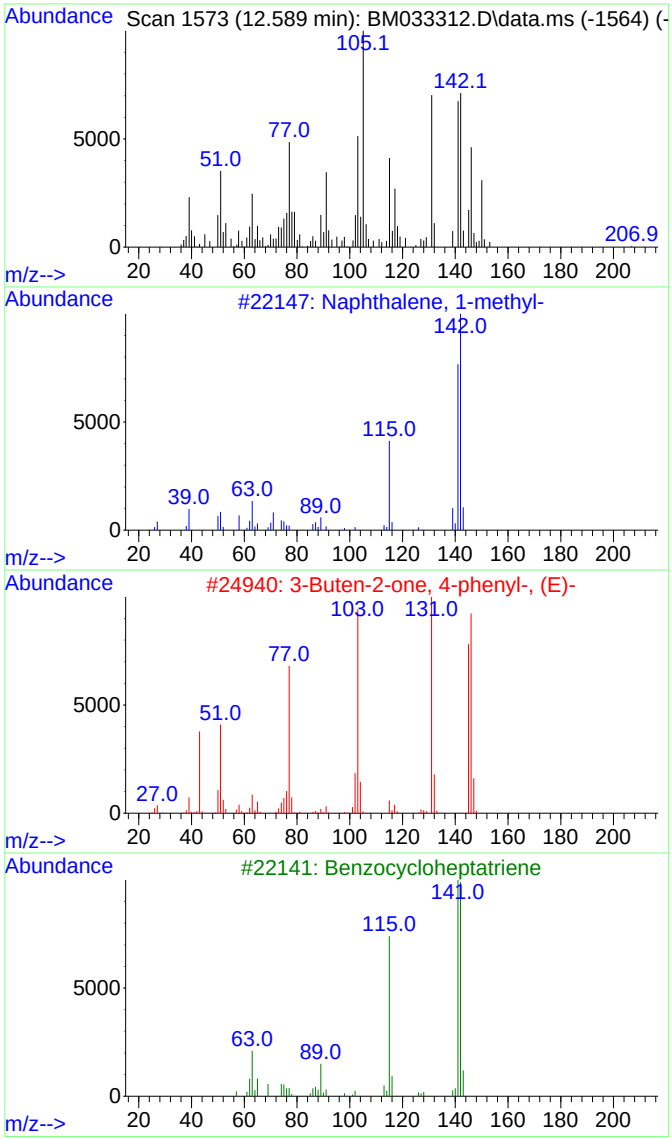
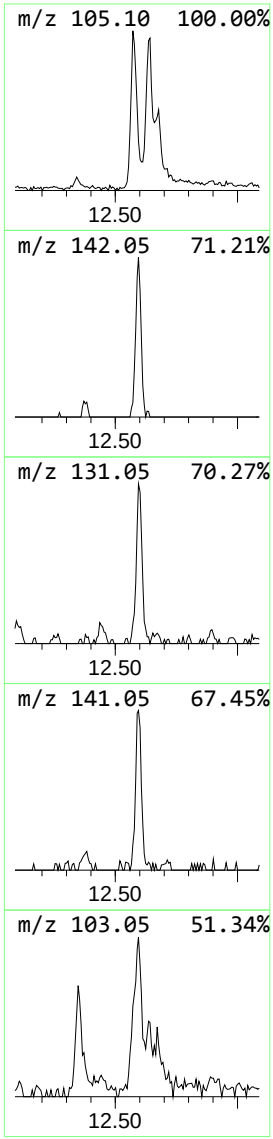
Peak Number 17 unknown12.589 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.589	4.09 ng	196771	Naphthalene-d8	10.719

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	46
2	3-Buten-2-one, 4-phenyl-, (E)-	146	C10H10O	001896-62-4	46
3	Benzocycloheptatriene	142	C11H10	000264-09-5	46
4	1-Methylindan-2-one	146	C10H10O	035587-60-1	45
5	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	38





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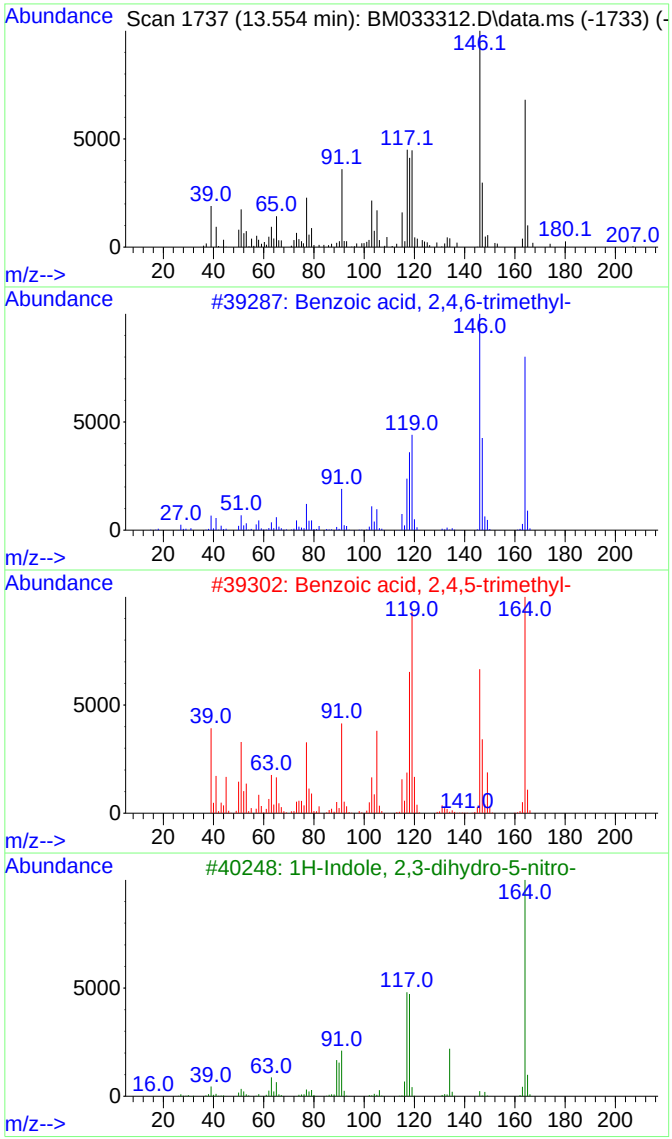
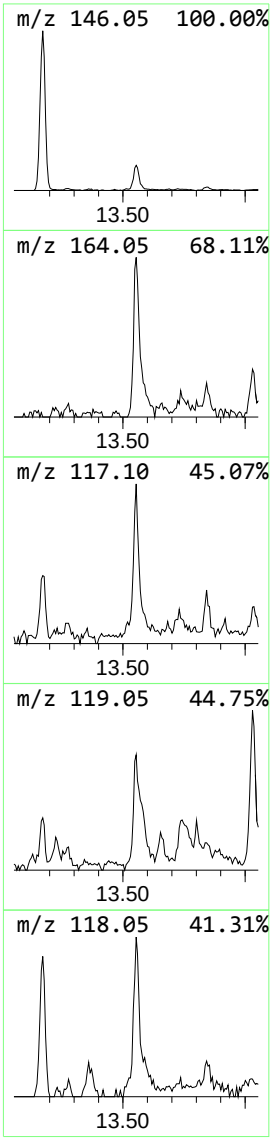
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.554	2.16 ng	126067	Acenaphthene-d10	14.548

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	93
2	Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	53
3	1H-Indole, 2,3-dihydro-5-nitro-	164	C8H8N2O2	032692-19-6	35
4	7-Benzofuranol, 2,3-dihydro-2,2-...	164	C10H12O2	001563-38-8	18
5	2-Propenoic acid, 3-(3-hydroxyph...	164	C9H8O3	000588-30-7	14





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Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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

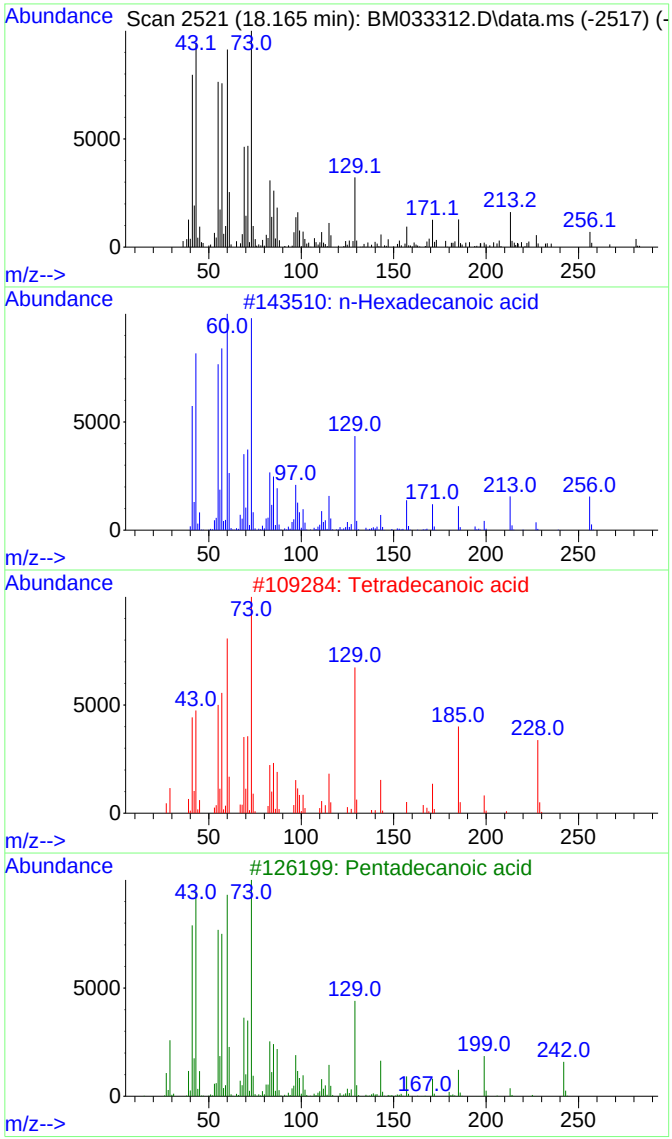
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

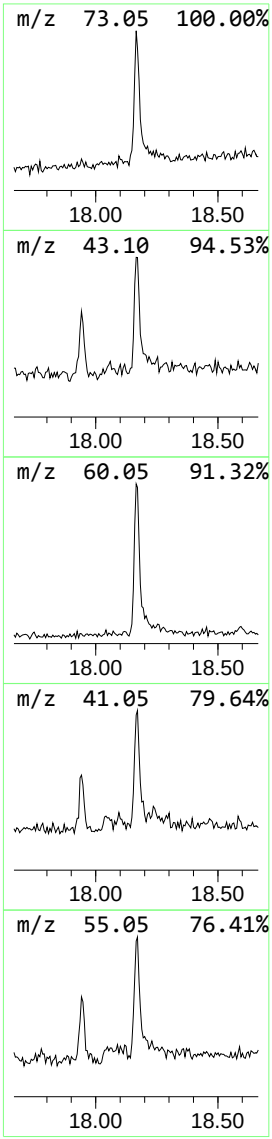
****

Peak Number 19 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.165	2.98 ng	208204	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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

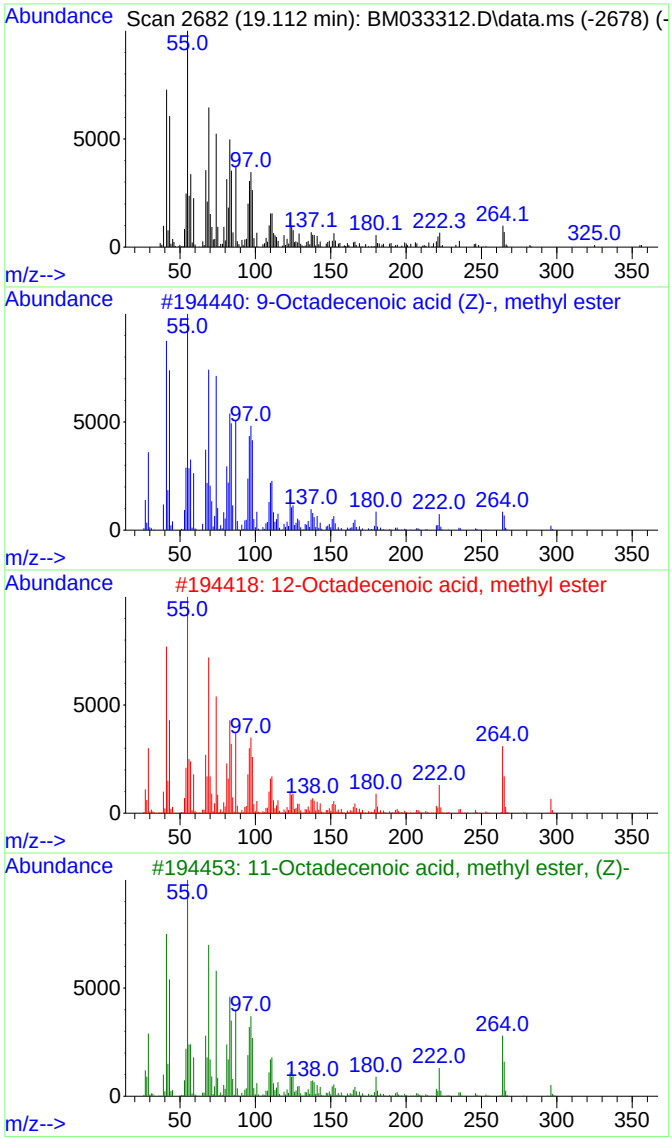
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

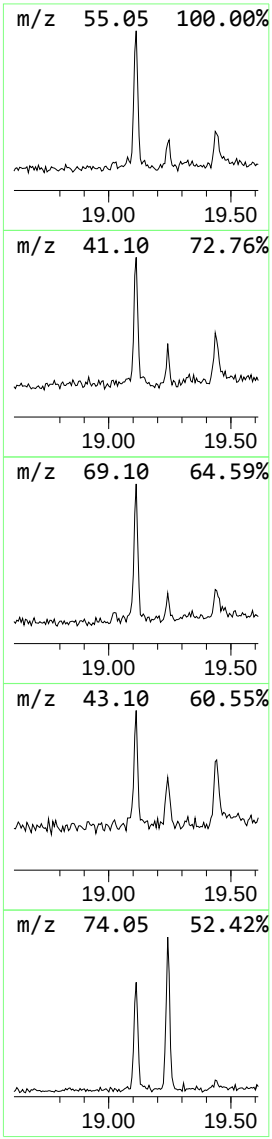
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 9-Octadecenoic acid (Z)-, m... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.112	2.99 ng	209409	Phenanthrene-d10	17.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	94
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	93
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033312.D
Acq On : 06 Dec 2021 14:59
Operator : CG/JU
Sample : M4917-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-35

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanol, 2-m...	3.654	8.9	ng	327532	1	7.925	737746	20.0
2-Pentanol, 2,4...	4.354	4.5	ng	166575	1	7.925	737746	20.0
Pentane, 2-butoxy-	4.419	2.9	ng	107806	1	7.925	737746	20.0
3-Pentanone, 2,...	4.449	3.5	ng	130803	1	7.925	737746	20.0
2-Pentanone, 4-...	5.043	6.0	ng	219567	1	7.925	737746	20.0
unknown6.119	6.119	2.1	ng	76781	1	7.925	737746	20.0
unknown7.325	7.325	3.0	ng	109247	1	7.925	737746	20.0
1-Methyl-1H-1,2...	8.019	2.4	ng	88392	1	7.925	737746	20.0
unknown8.072	8.072	6.4	ng	237510	1	7.925	737746	20.0
Hexanoic acid, ...	8.195	18.9	ng	697754	1	7.925	737746	20.0
Indane	8.295	7.1	ng	260892	1	7.925	737746	20.0
unknown8.919	8.919	19.7	ng	727960	1	7.925	737746	20.0
unknown8.989	8.989	18.5	ng	682633	1	7.925	737746	20.0
unknown9.719	9.719	5.5	ng	265078	2	10.719	962792	20.0
Ethanol, 2-(2-b...	10.495	7.2	ng	348325	2	10.719	962792	20.0
4,5-Octanediol,...	12.354	2.8	ng	136788	2	10.719	962792	20.0
unknown12.589	12.589	4.1	ng	196771	2	10.719	962792	20.0
Benzoic acid, 2...	13.554	2.2	ng	126067	3	14.548	1166190	20.0
n-Hexadecanoic ...	18.165	3.0	ng	208204	4	17.289	1399490	20.0
9-Octadecenoic ...	19.112	3.0	ng	209409	4	17.289	1399490	20.0