LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138448.D
Acq On : 03 Jul 2024 16:11
Operator : CG\JU
Sample : P3129-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT4259

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_F\Methods\8270-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	21	rVB	1801565	2326918	95.74%	12.658%
2	5.087	506	510	518	rVB	264230	292310	12.03%	1.590%
3	5.498	575	580	583	rBV	2320197	2211379	90.99%	12.029%
4	6.504	746	751	762	rBV	2635774	2430345	100.00%	13.220%
5	6.869	810	813	817	rBV	907280	706764	29.08%	3.845%
6	6.928	820	823	835	rBV	517771	457959	18.84%	2.491%
7	7.434	904	909	912	rVB	1646087	1456528	59.93%	7.923%
8	8.151	1027	1031	1034	rBV	1029475	809700	33.32%	4.405%
9	9.104	1189	1193	1196	rBV4	43767	78872	3.25%	0.429%
10	9.228	1209	1214	1217	rBV	2289153	2059925	84.76%	11.205%
11	9.263	1217	1220	1223	rBV4	99007	86598	3.56%	0.471%
12	9.304	1223	1227	1230	rBV2	223344	296950	12.22%	1.615%
13	9.539	1264	1267	1269	rBV3	234587	253950	10.45%	1.381%
14	9.581	1272	1274	1277	rVB4	161057	162952	6.70%	0.886%
15	9.628	1277	1282	1284	rBV3	348424	543102	22.35%	2.954%
16	9.651	1284	1286	1289	rVV3	159830	189024	7.78%	1.028%
17	9.722	1294	1298	1301	rBV2	796452	851007	35.02%	4.629%
18	9.775	1304	1307	1310	rBV5	344921	506720	20.85%	2.756%
19	9.816	1311	1314	1316	rBV4	376670	420541	17.30%	2.288%
20	9.904	1324	1329	1332	rBV2	914170	1195573	49.19%	6.504%
21	10.169	1371	1374	1376	rBV3	376436	519322	21.37%	2.825%
22	10.316	1397	1399	1401	rBV	568306	526860	21.68%	2.866%

Sum of corrected areas: 18383299

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Instrument :
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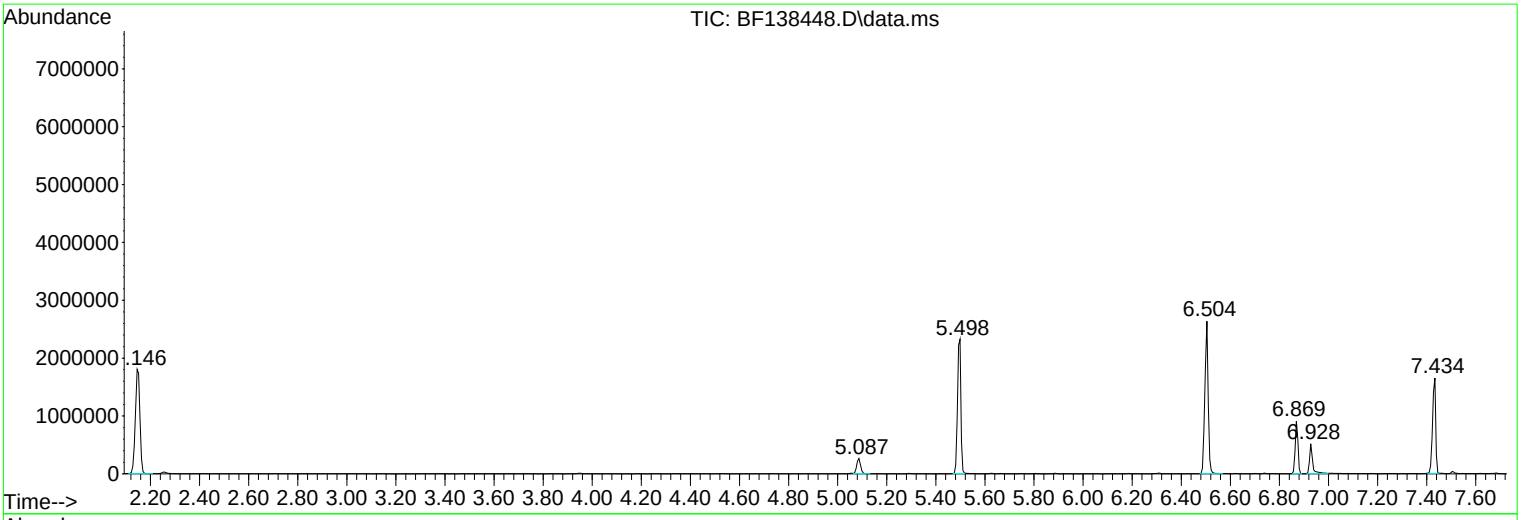
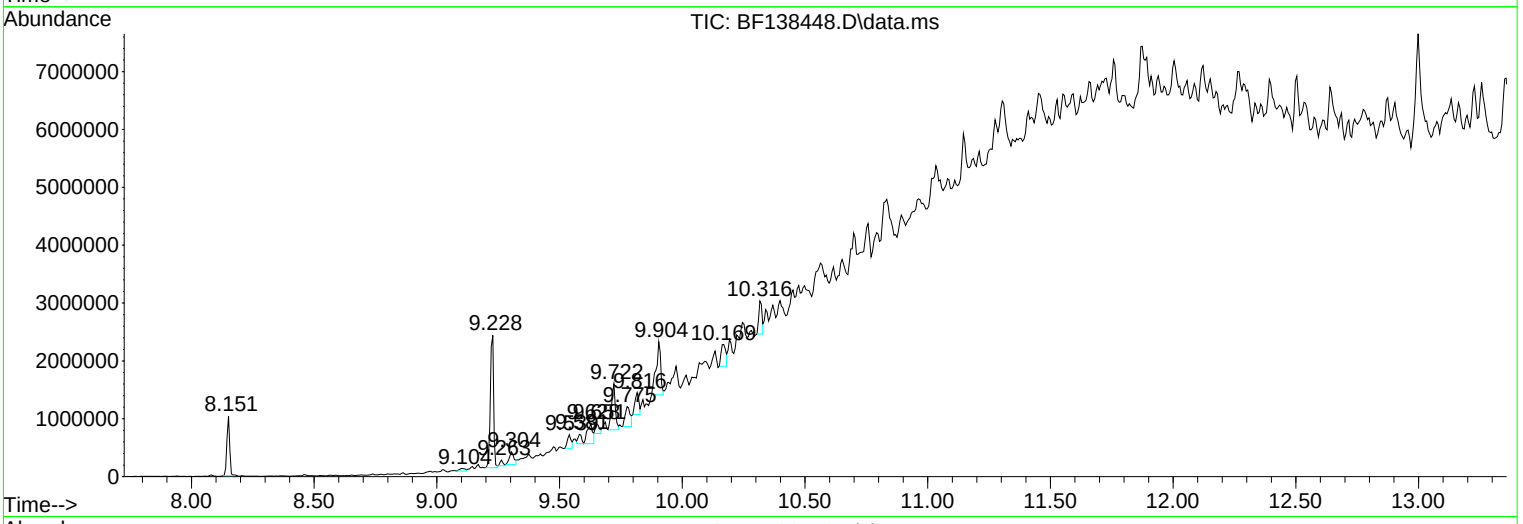
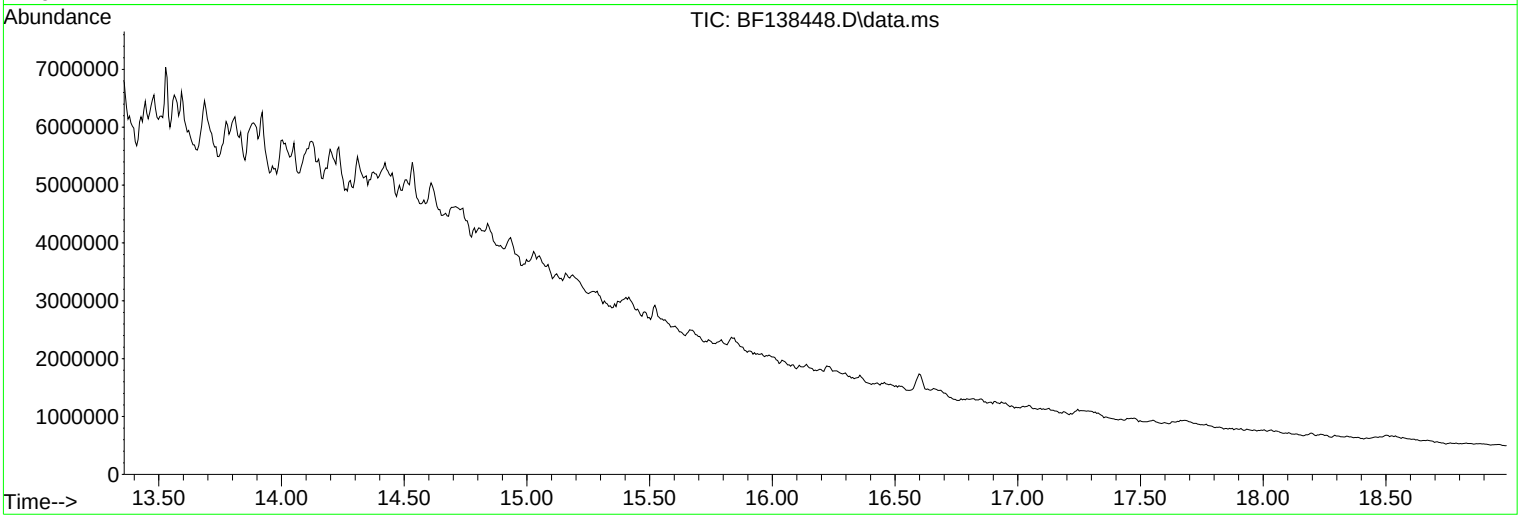
ClientSampleId :
RT4259

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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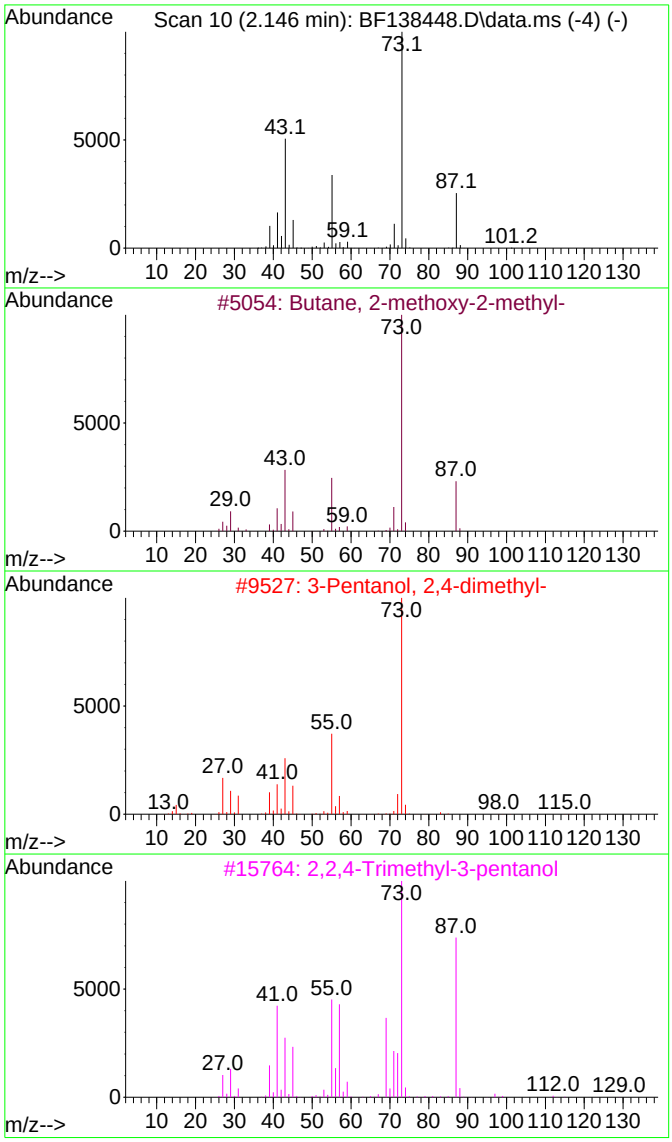
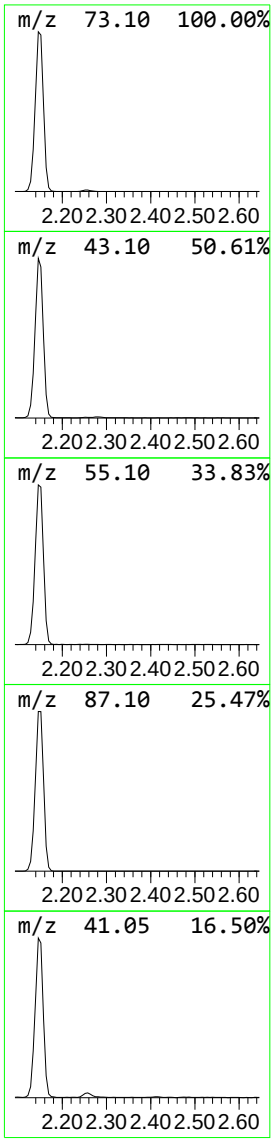
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	65.85 ng	2326920	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Operator : CG\JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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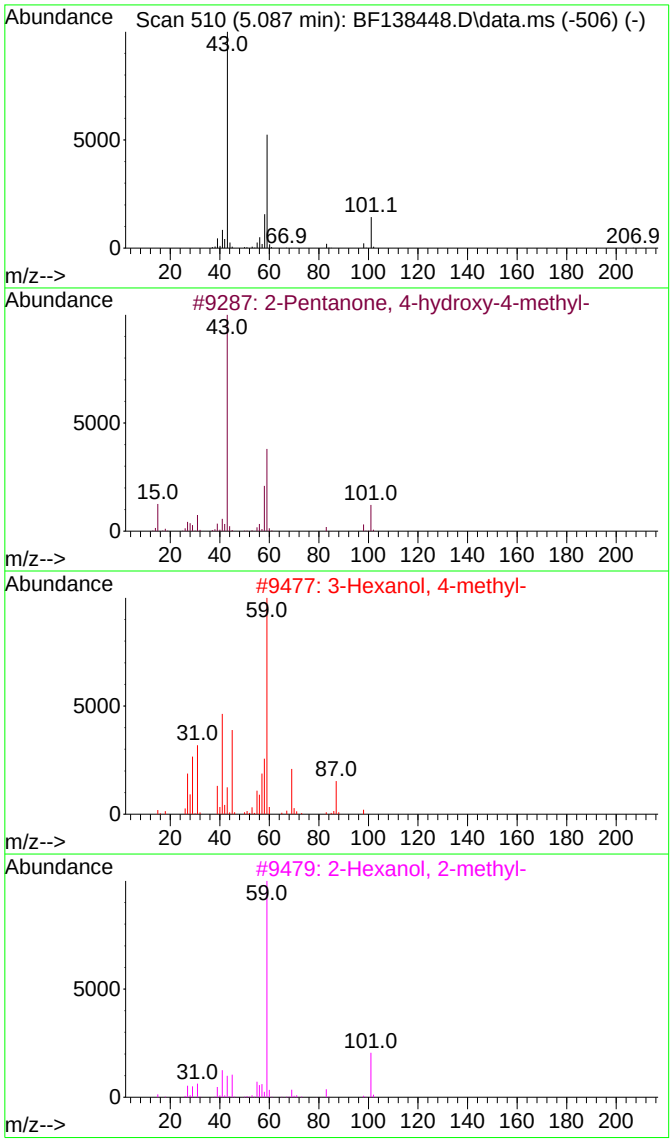
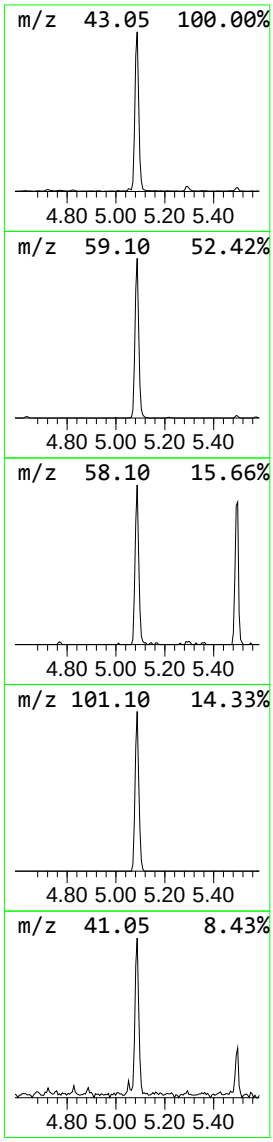
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	8.27 ng	292310	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Sample : P3129-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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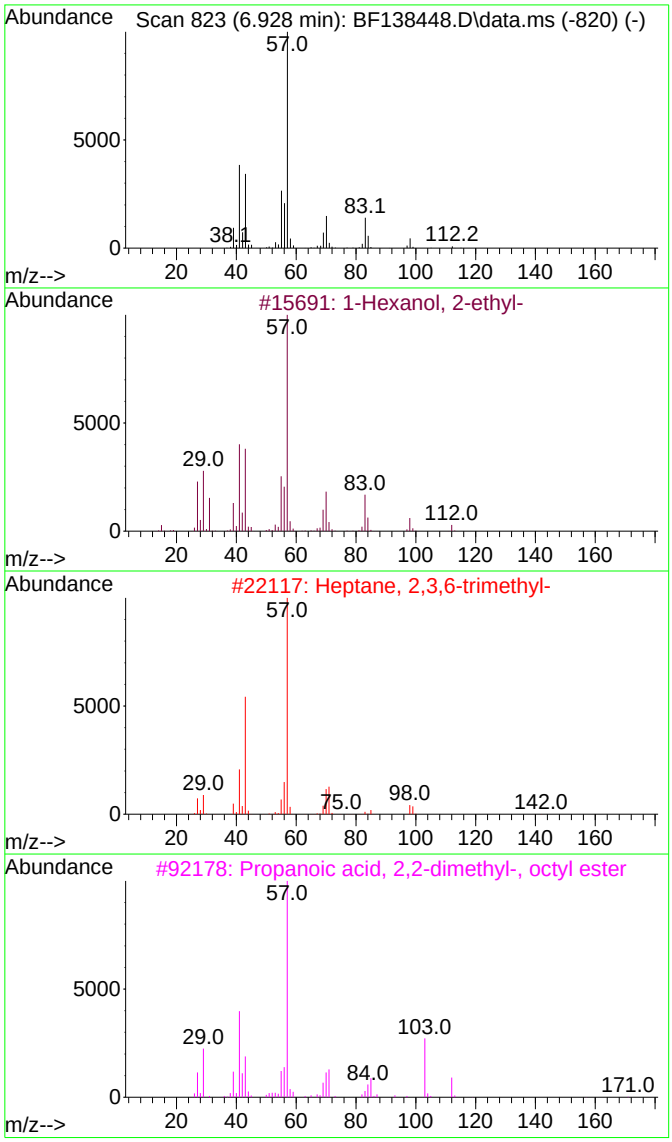
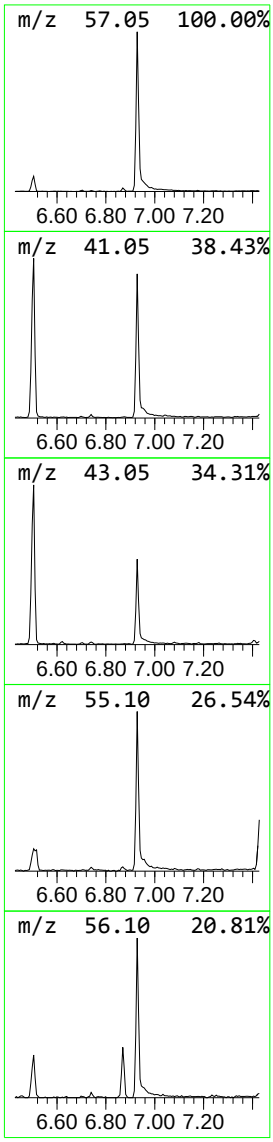
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	12.96 ng	457959	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
3	Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	64
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56





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Sample : P3129-01
Misc :
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Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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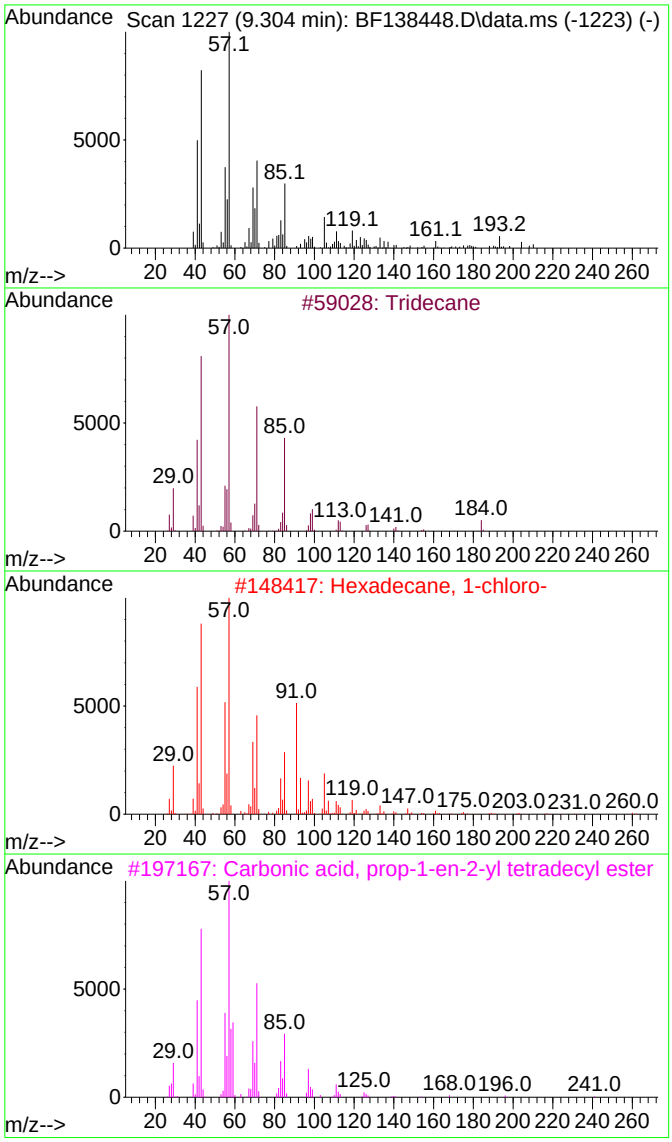
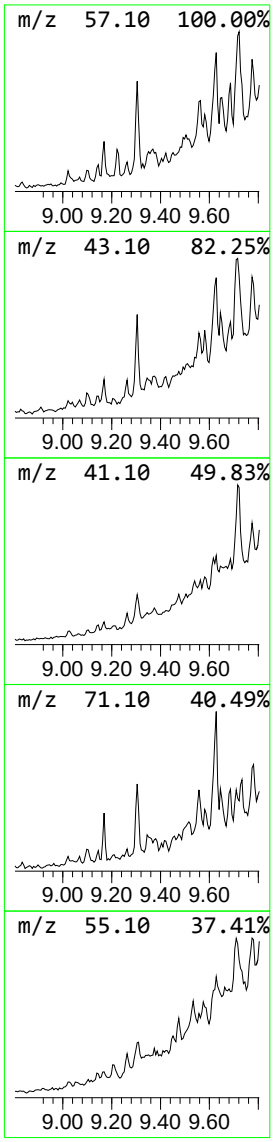
****

Peak Number 4 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	4.97 ng	296950	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	72
2	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	64
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	64
4	Tetradecane	198	C14H30	000629-59-4	62
5	Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	53





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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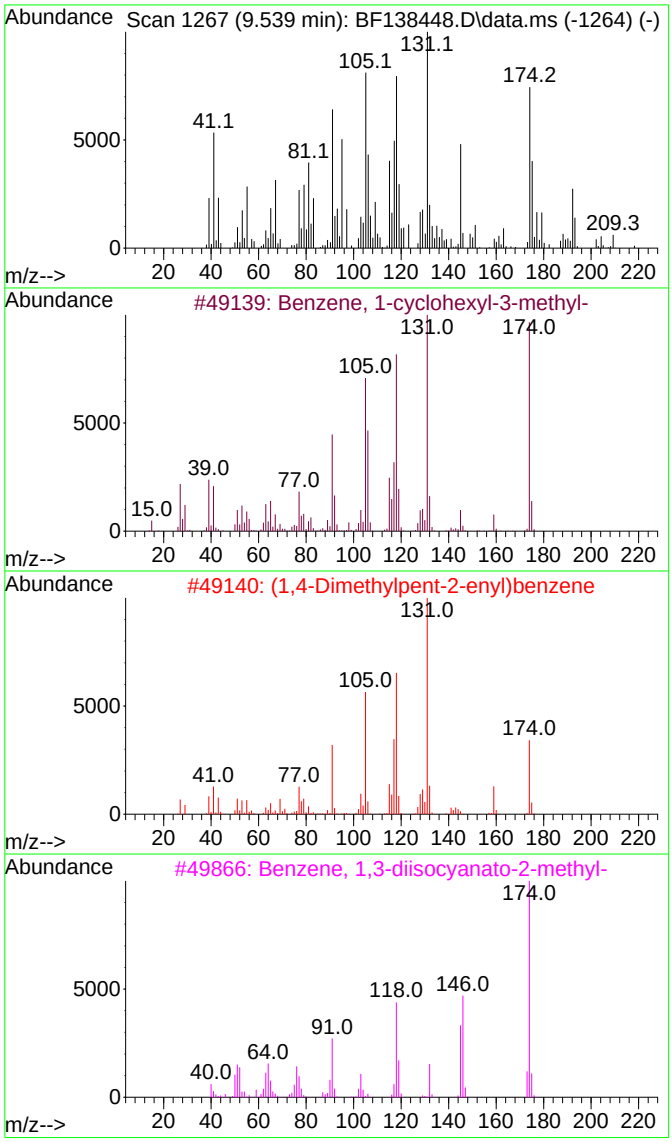
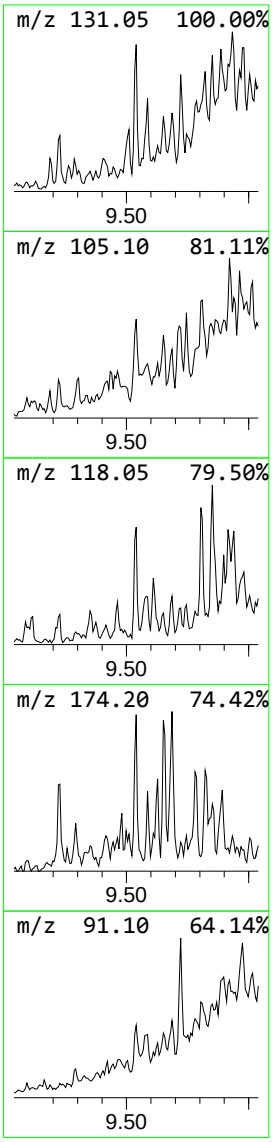
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-cyclohexyl-3-met... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.539	4.25 ng	253950	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	64
2	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	53
3	Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	46
4	Benzenemethanamine, 3-(trifluoro...	175	C8H8F3N	002740-83-2	22
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	15





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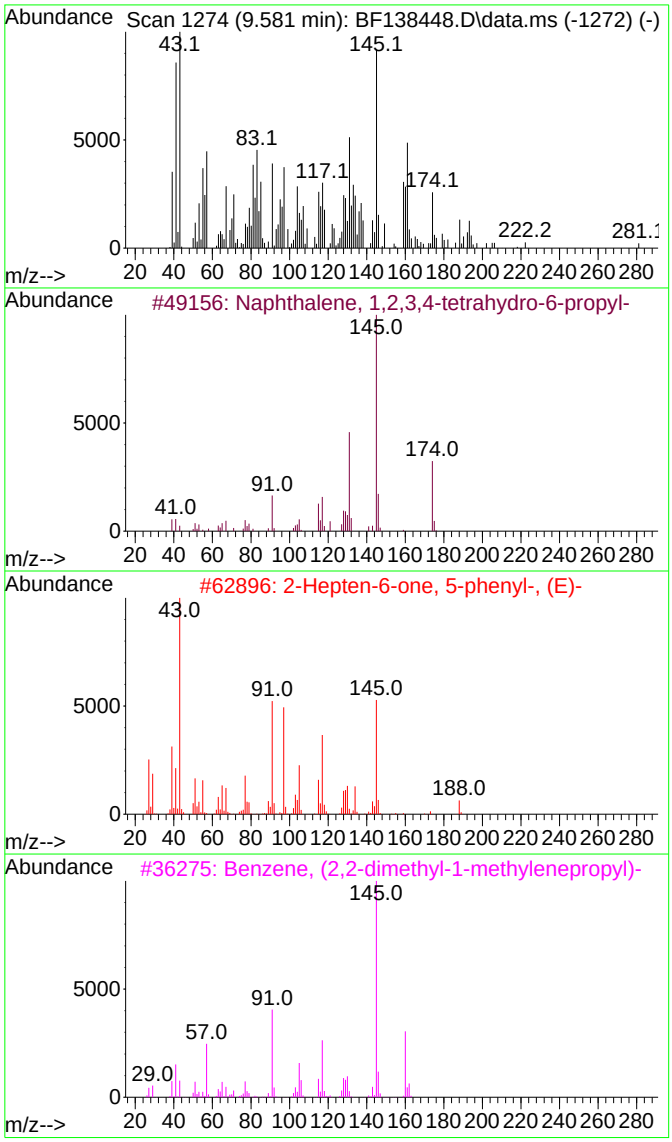
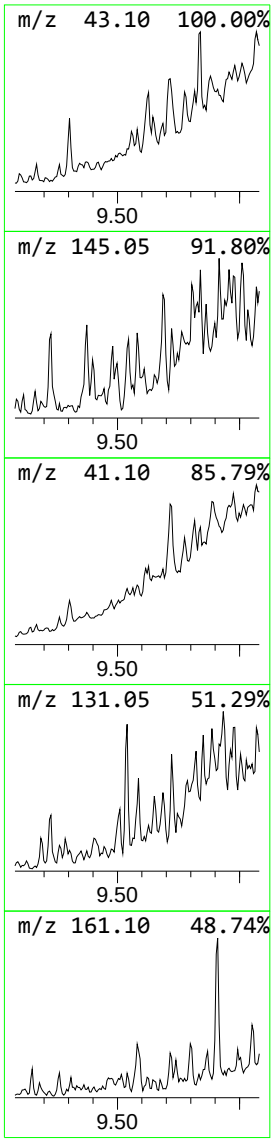
****

Peak Number 6 unknown9.581 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.581	2.73 ng	162952	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	042775-77-9	41
2	2-Hepten-6-one, 5-phenyl-, (E)-	188	C13H16O	1000159-12-2	38
3	Benzene, (2,2-dimethyl-1-methyle...	160	C12H16	005676-29-9	38
4	Dispiro[4.2.4.2]tetradeca-6,13-d...	188	C14H20	078578-90-2	38
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	38





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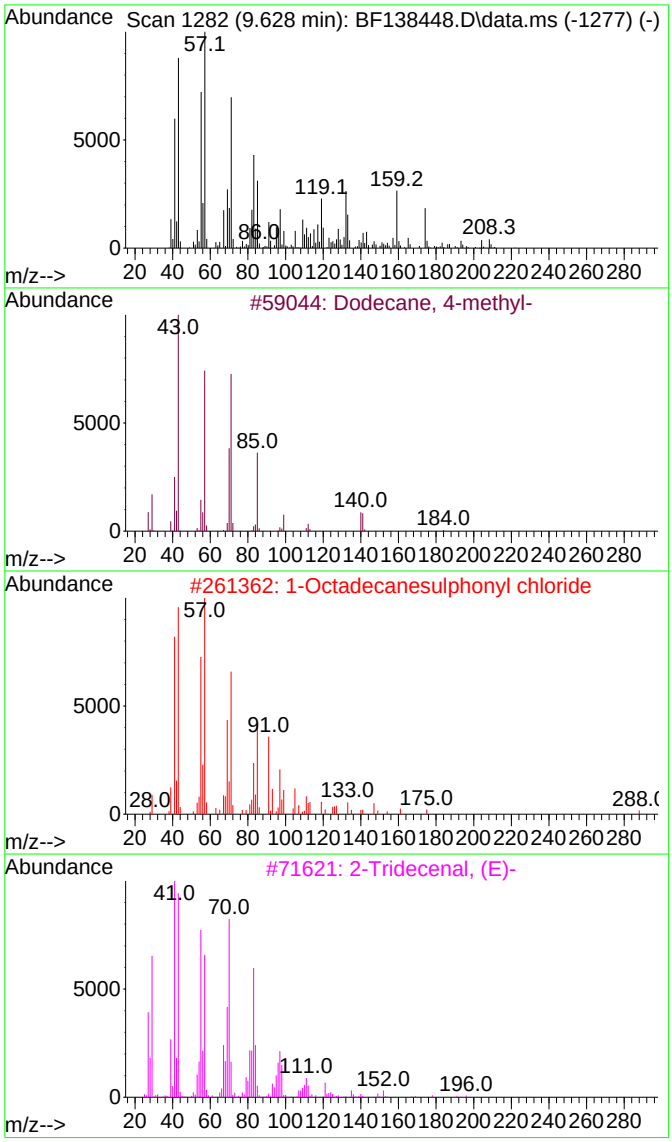
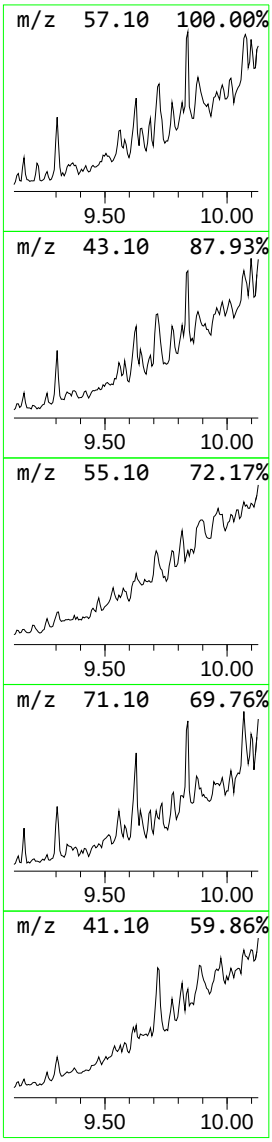
****

Peak Number 7 unknown9.628 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.628	9.09 ng	543102	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4-methyl-	184	C13H28	006117-97-1	35
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	25
3	2-Tridecenal, (E)-	196	C13H24O	007069-41-2	25
4	Nonane	128	C9H20	000111-84-2	25
5	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	25





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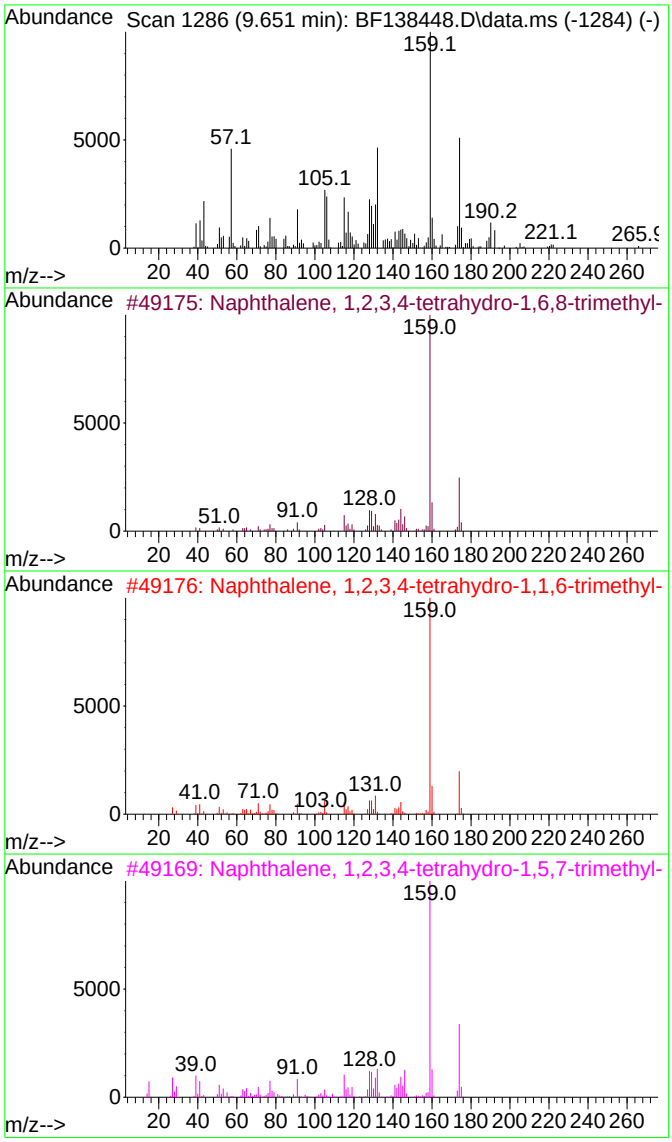
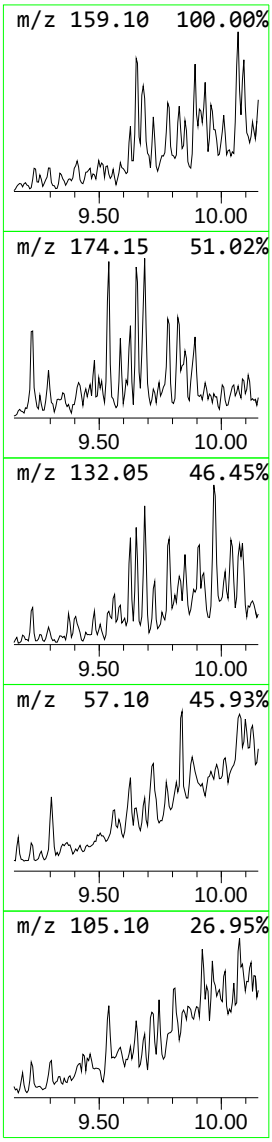
****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.651	3.16 ng	189024	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	93
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	93
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-55-0	92
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	022824-32-4	81
5	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-17-7	76





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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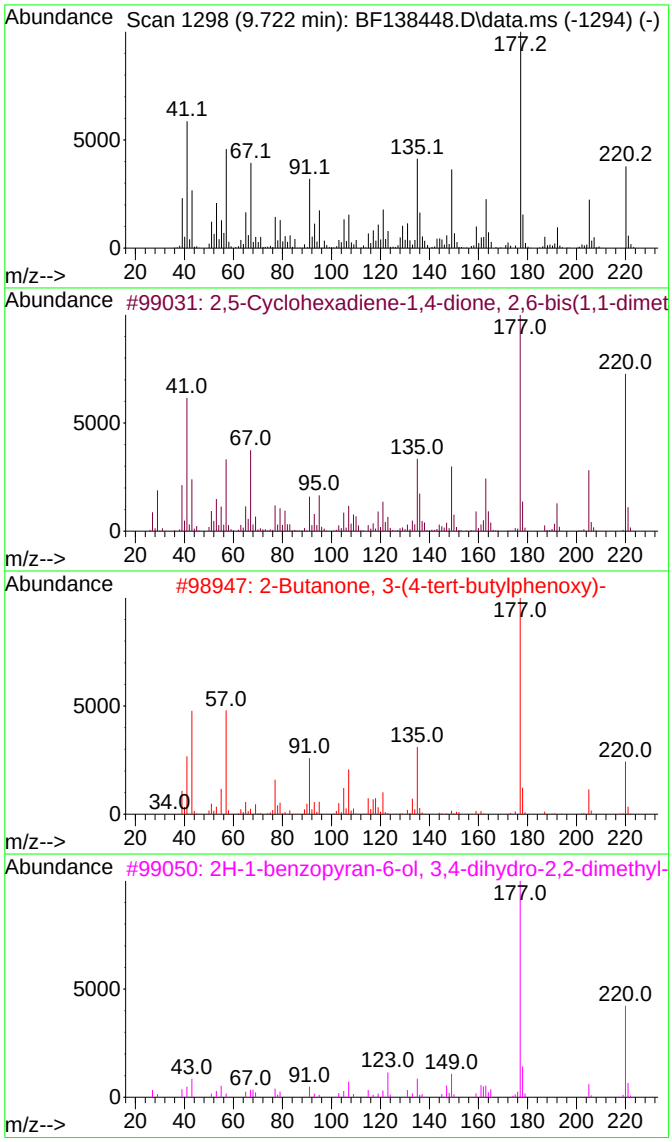
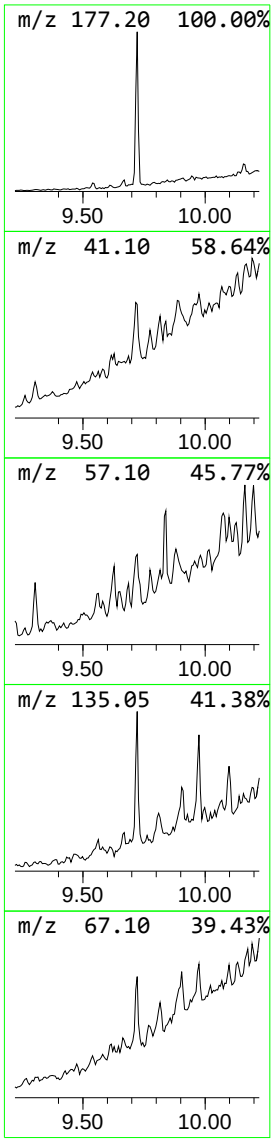
****
Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	14.24 ng	851007	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	55
3	2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	50
4	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	45
5	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	45





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Data File : BF138448.D
Acq On : 03 Jul 2024 16:11
Operator : CG\JU
Sample : P3129-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT4259

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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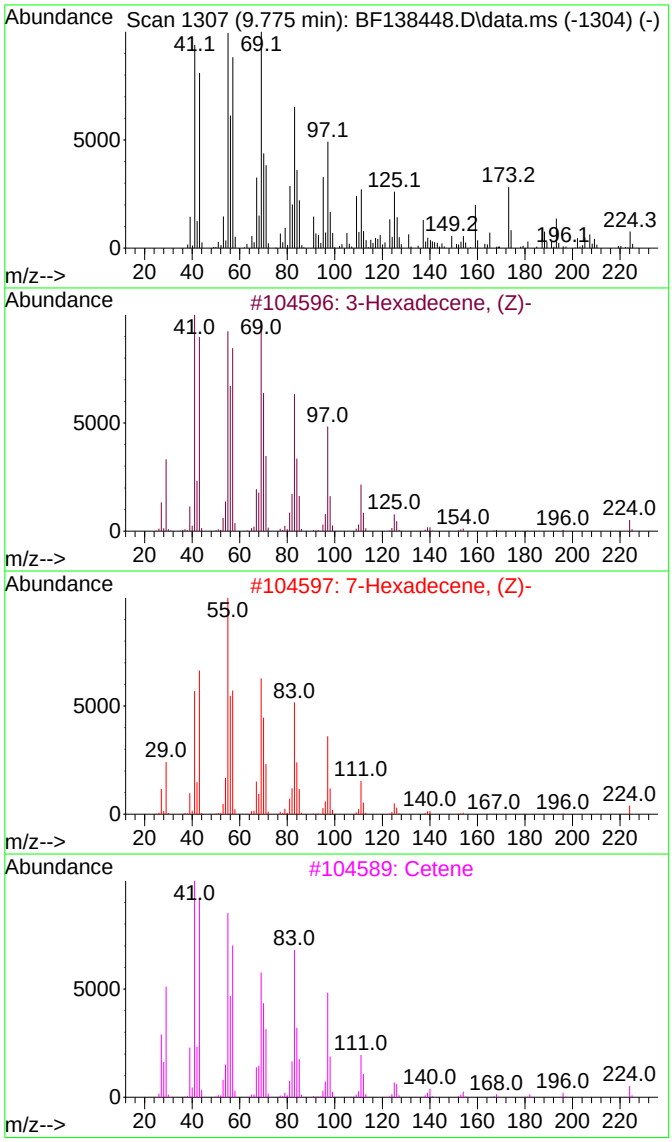
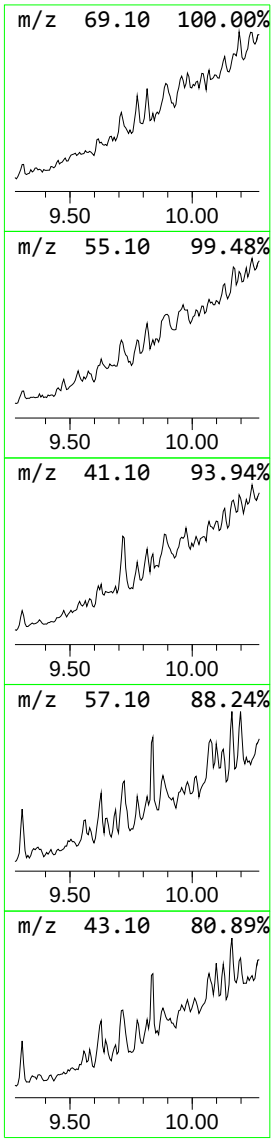
Peak Number 10 3-Hexadecene, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.775	8.48 ng	506720	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	83
2	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	78
3	Cetene	224	C16H32	000629-73-2	60
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1010282-97-2	53
5	1-Undecene, 8-methyl-	168	C12H24	074630-40-3	50





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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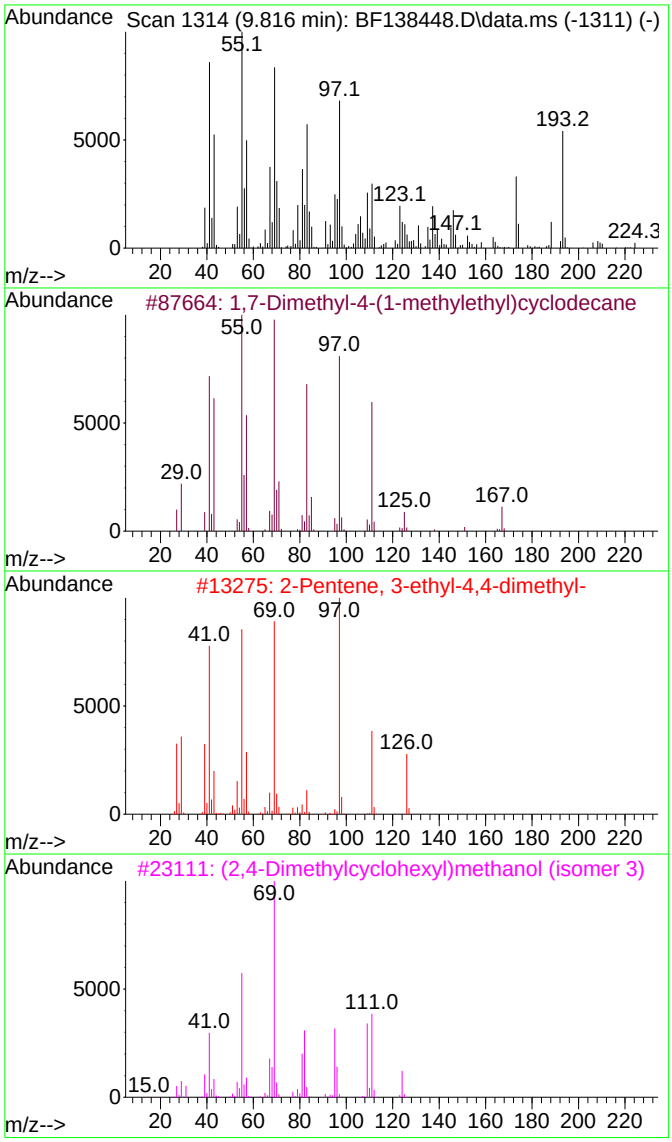
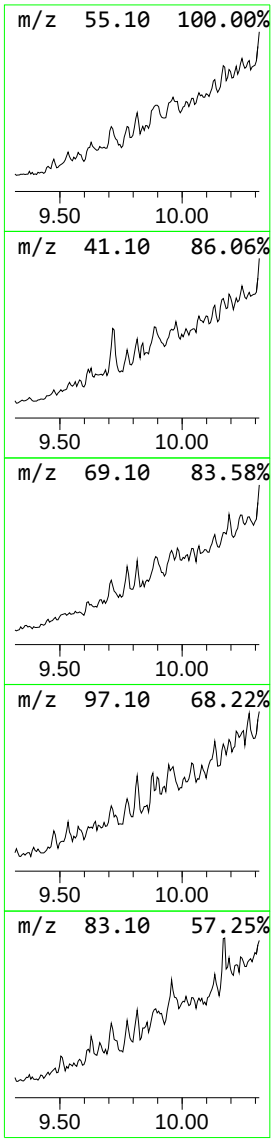
Peak Number 11 unknown9.816 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	7.03 ng	420541	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	38
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	35
3	(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-8	27
4	2-Butenamide, 2,3-dimethyl-N-phe...	189	C12H15NO	024735-54-4	27
5	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	25





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Data File : BF138448.D
Acq On : 03 Jul 2024 16:11
Operator : CG\JU
Sample : P3129-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT4259

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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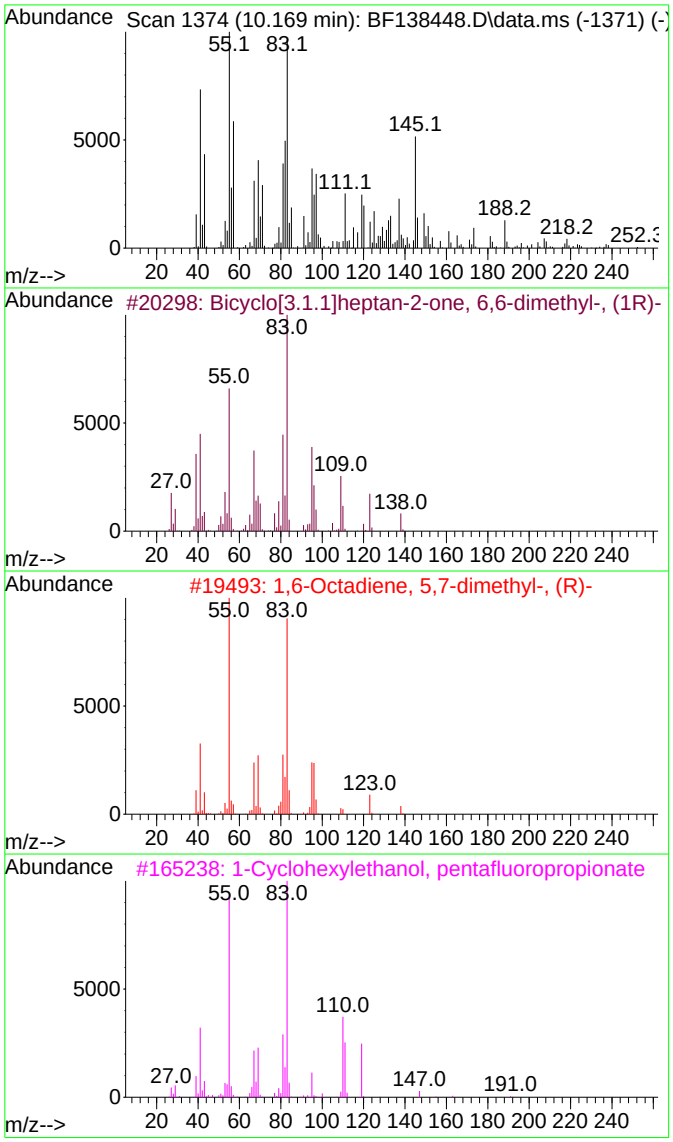
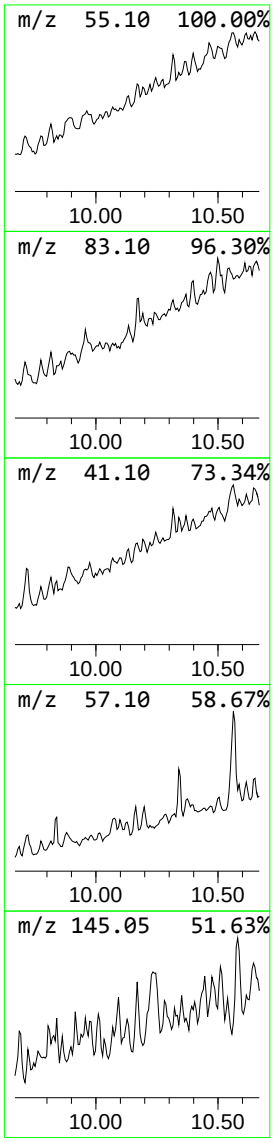
Peak Number 12 unknown10.169 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.169	8.69 ng	519322	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	038651-65-9	42
2	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	41
3	1-Cyclohexylethanol, pentafluoro...	274	C11H15F5O2	1000365-50-1	35
4	Cyclobutanecarboxylic acid, oct-...	210	C13H22O2	1000299-13-2	25
5	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	22





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Data File : BF138448.D
Acq On : 03 Jul 2024 16:11
Operator : CG\JU
Sample : P3129-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT4259

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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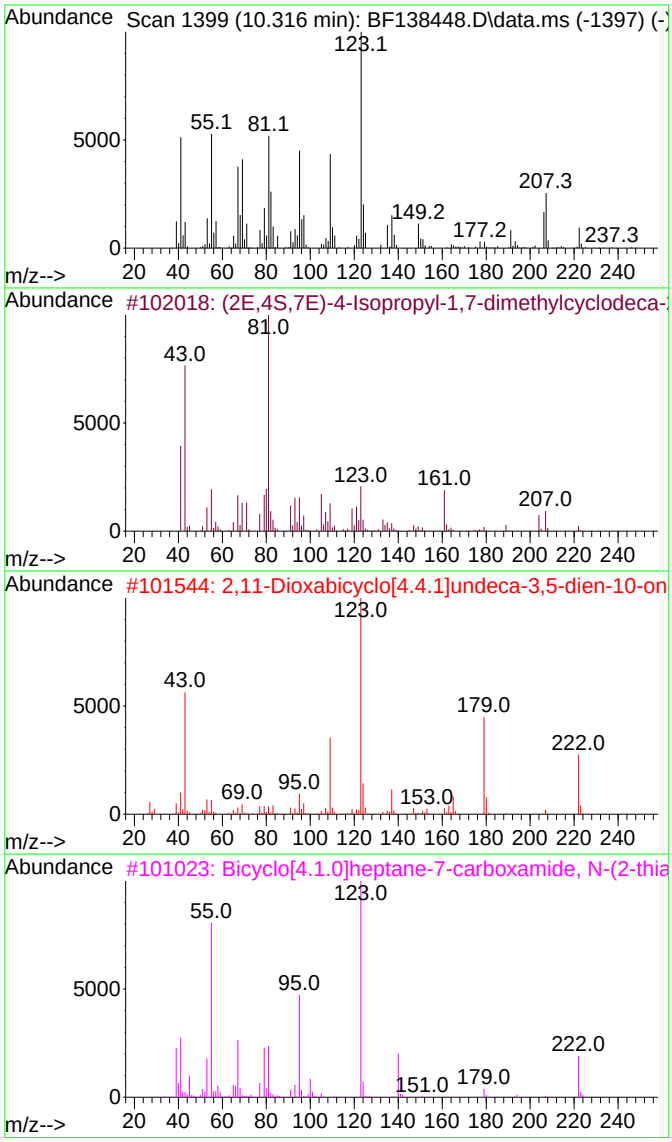
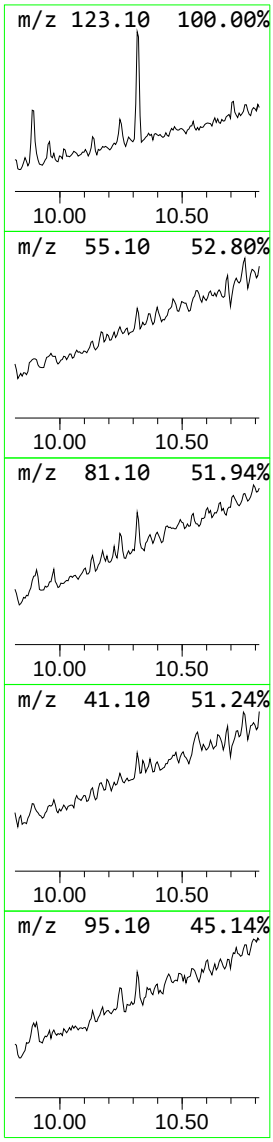
Peak Number 13 (2E,4S,7E)-4-Isopropyl-1,7-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	8.81 ng	526860	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2E,4S,7E)-4-Isopropyl-1,7-dimet...	222	C15H26O	198991-79-6	53
2	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	47
3	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	46
4	3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1010277-78-0	38
5	N-[(4-Fluorophenyl)carbonyl]glycine	197	C9H8FNO3	000366-79-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138448.D
Acq On : 03 Jul 2024 16:11
Operator : CG\JU
Sample : P3129-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT4259

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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
Butane, 2-metho...	2.146	65.8	ng	2326920	1	6.869	706764	20.0
2-Pentanone, 4-...	5.087	8.3	ng	292310	1	6.869	706764	20.0
1-Hexanol, 2-et...	6.928	13.0	ng	457959	1	6.869	706764	20.0
Tridecane	9.304	5.0	ng	296950	3	9.904	1195570	20.0
Benzene, 1-cycl...	9.539	4.3	ng	253950	3	9.904	1195570	20.0
unknown9.581	9.581	2.7	ng	162952	3	9.904	1195570	20.0
unknown9.628	9.628	9.1	ng	543102	3	9.904	1195570	20.0
Naphthalene, 1,...	9.651	3.2	ng	189024	3	9.904	1195570	20.0
2,5-Cyclohexadi...	9.722	14.2	ng	851007	3	9.904	1195570	20.0
3-Hexadecene, (Z)-	9.775	8.5	ng	506720	3	9.904	1195570	20.0
unknown9.816	9.816	7.0	ng	420541	3	9.904	1195570	20.0
unknown10.169	10.169	8.7	ng	519322	3	9.904	1195570	20.0
(2E,4S,7E)-4-Is...	10.316	8.8	ng	526860	3	9.904	1195570	20.0