LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047564.D
Acq On : 18 Sep 2024 20:25
Operator : RC/JU
Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
365-351-294

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-BM091424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047564.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	311	319	329	rVB	208803	313877	2.72%	0.483%
2	5.422	391	397	406	rBV	3873131	5563624	48.14%	8.556%
3	7.010	660	667	682	rVB	3897900	5976268	51.71%	9.191%
4	7.851	803	810	816	rVB	1110086	1767876	15.30%	2.719%
5	9.004	989	1006	1012	rBV	2180878	3801621	32.90%	5.847%
6	9.334	1057	1062	1069	rVB4	78724	193333	1.67%	0.297%
7	9.510	1085	1092	1098	rBV4	114688	246724	2.13%	0.379%
8	9.569	1098	1102	1109	rVB6	118351	230365	1.99%	0.354%
9	9.739	1123	1131	1135	rBV5	94632	185852	1.61%	0.286%
10	9.840	1143	1148	1156	rBV5	141695	259797	2.25%	0.400%
11	10.645	1277	1285	1290	rBV	1420360	2448458	21.19%	3.765%
12	10.698	1290	1294	1299	rVB	188458	303280	2.62%	0.466%
13	10.822	1311	1315	1321	rVB	378251	554728	4.80%	0.853%
14	11.151	1367	1371	1378	rBV5	122103	229674	1.99%	0.353%
15	11.357	1396	1406	1414	rBV9	171893	468562	4.05%	0.721%
16	11.692	1457	1463	1467	rBV	288351	543822	4.71%	0.836%
17	11.945	1502	1506	1511	rBV4	105454	178766	1.55%	0.275%
18	12.304	1564	1567	1572	rVB3	221680	360893	3.12%	0.555%
19	12.392	1578	1582	1588	rBV4	134504	231021	2.00%	0.355%
20	12.992	1680	1684	1688	rBV5	77308	162727	1.41%	0.250%
21	13.039	1688	1692	1696	rVV2	229047	327096	2.83%	0.503%
22	13.104	1697	1703	1717	rVB	4979558	7318514	63.33%	11.255%
23	13.280	1729	1733	1736	rBV5	106451	180999	1.57%	0.278%
24	13.916	1837	1841	1848	rBV3	217418	288143	2.49%	0.443%
25	13.980	1848	1852	1856	rVB	162586	205858	1.78%	0.317%
26	14.322	1907	1910	1917	rVB3	158979	245904	2.13%	0.378%
27	14.480	1929	1937	1944	rBV	1851973	2853853	24.70%	4.389%
28	15.222	2058	2063	2068	rBV	746738	994244	8.60%	1.529%
29	15.833	2162	2167	2172	rBV	1078755	1480489	12.81%	2.277%
30	15.963	2183	2189	2194	rBV	3765258	5176600	44.79%	7.961%
31	17.215	2398	2402	2407	rBV	2312240	3243745	28.07%	4.989%
32	19.833	2843	2847	2854	rVB	9070068	11556217	100.00%	17.772%
33	21.445	3118	3121	3126	rVB	2506734	3713162	32.13%	5.710%
34	24.480	3630	3637	3647	rVB	1372063	3417444	29.57%	5.256%

Sum of corrected areas: 65023536

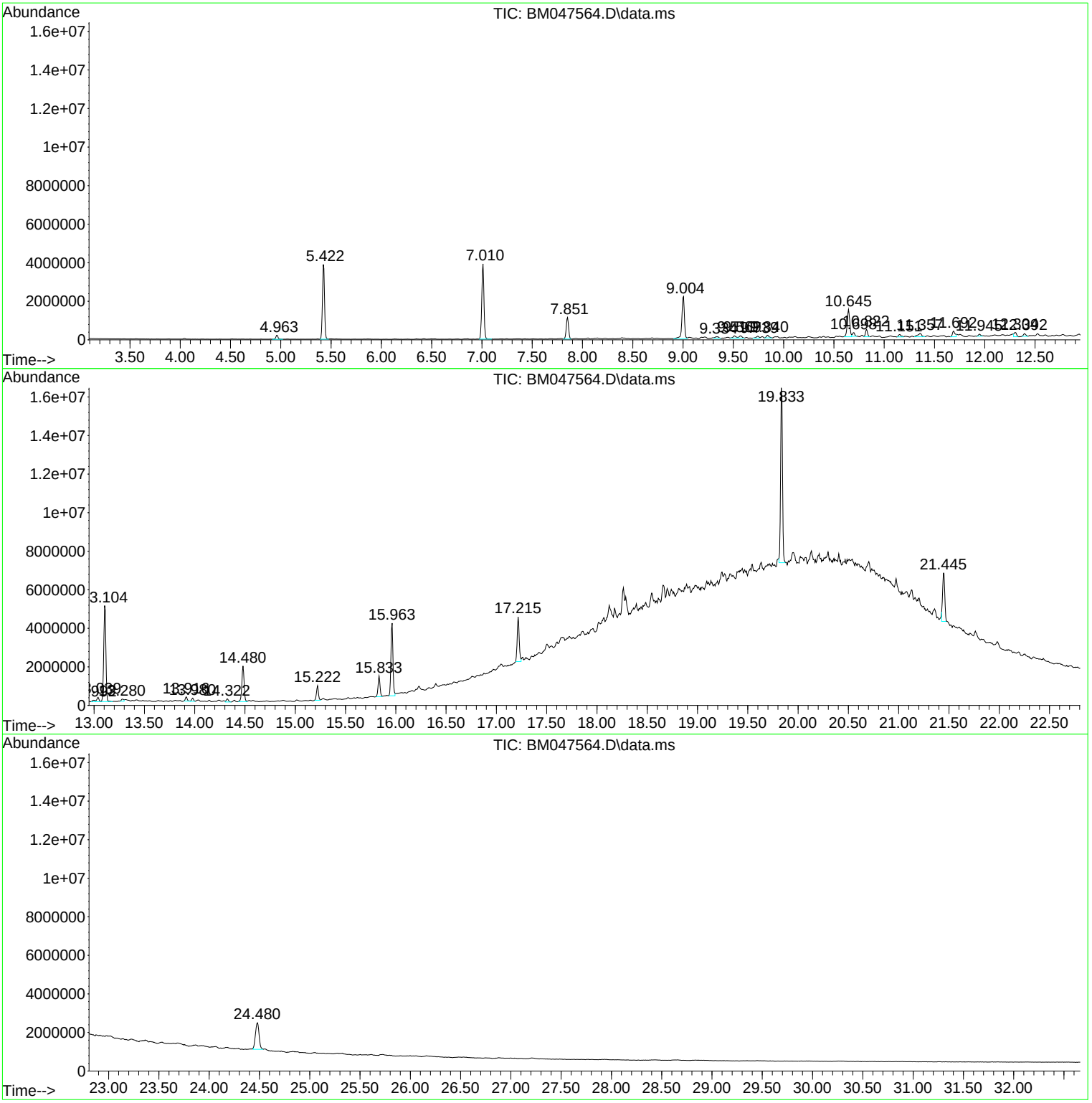
Instrument :
BNA_M
ClientSampleId :
365-351-294

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047564.D
Acq On : 18 Sep 2024 20:25
Operator : RC/JU
Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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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TIC Library : C:\Database\NIST20.L
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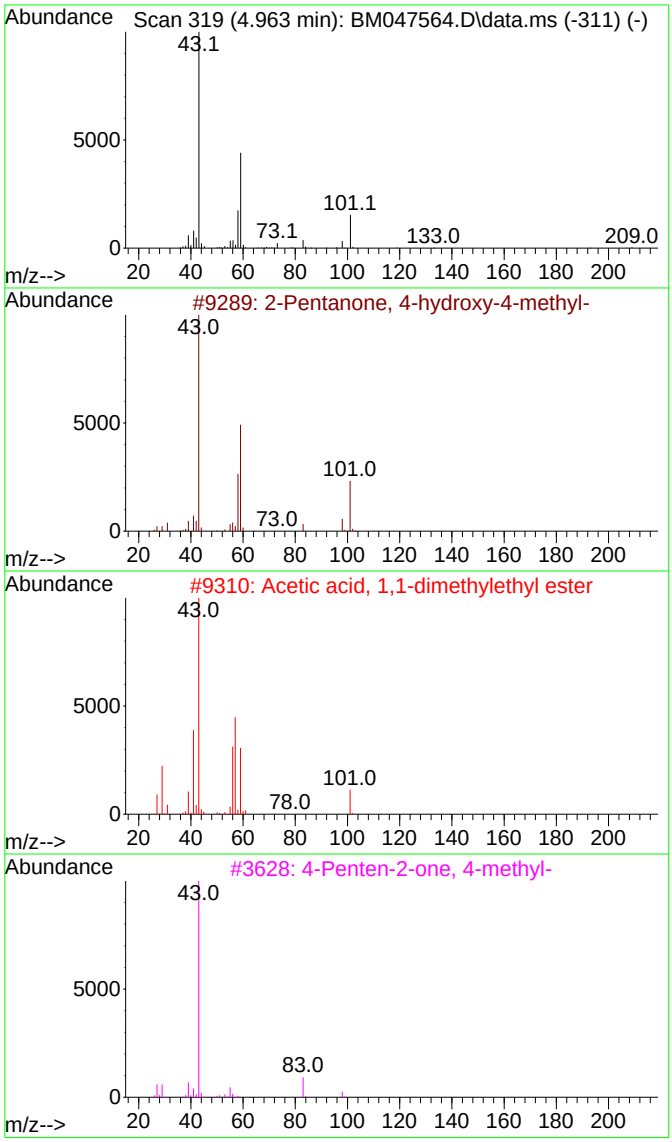
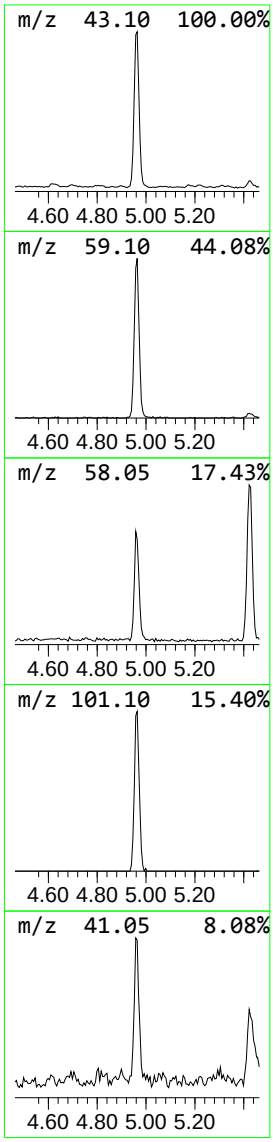
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	3.55 ng	313877	1,4-Dichlorobenzene-d4	7.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	14
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Operator : RC/JU
Sample : P4089-01
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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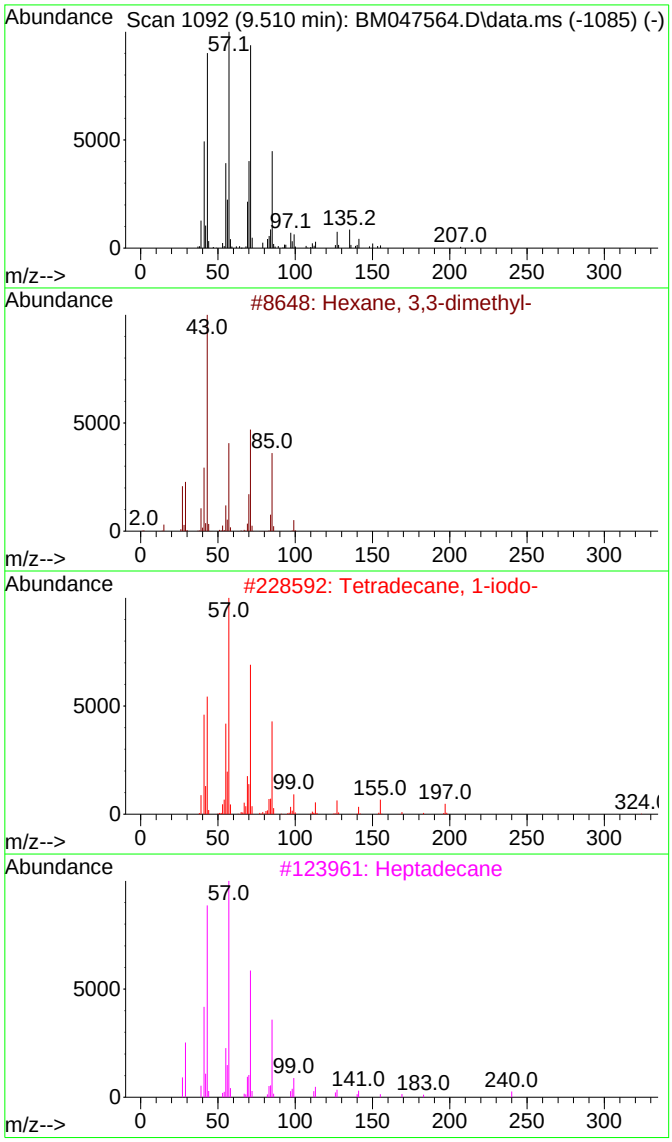
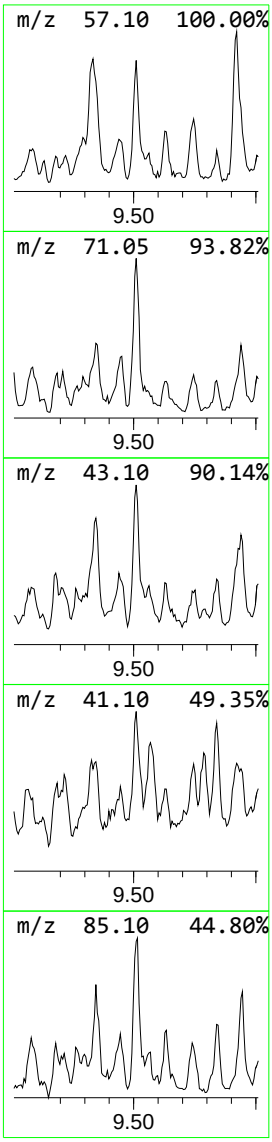
****

Peak Number 2 Hexane, 3,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.510	2.02 ng	246724	Naphthalene-d8	10.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	72
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
3	Heptadecane	240	C17H36	000629-78-7	59
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	53
5	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	50





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Sample : P4089-01
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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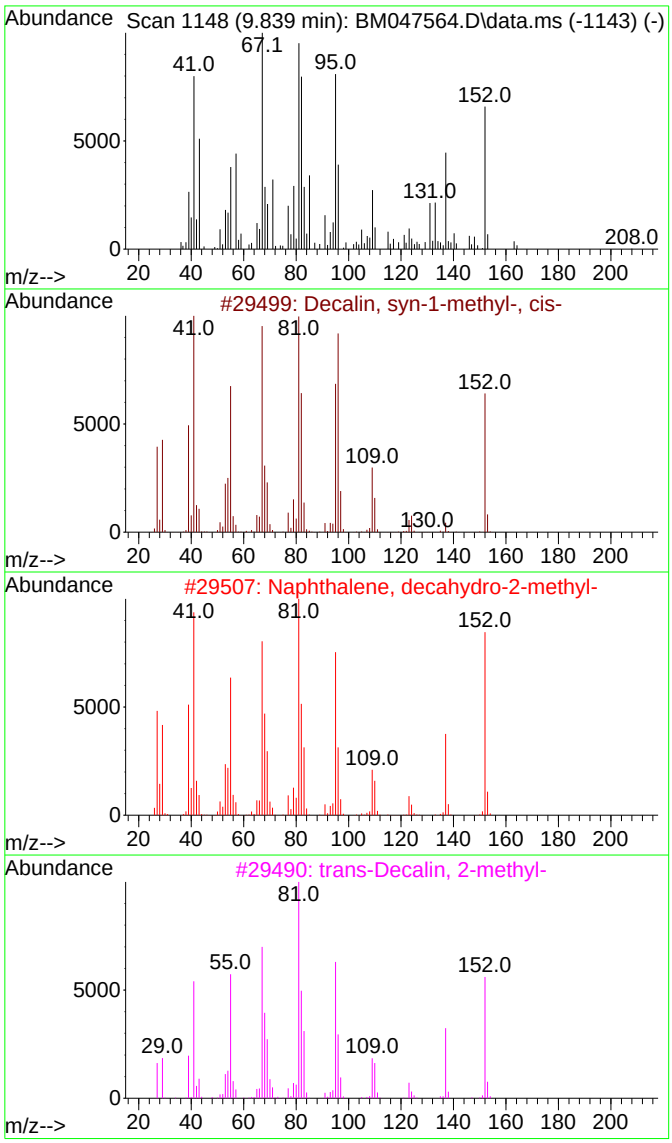
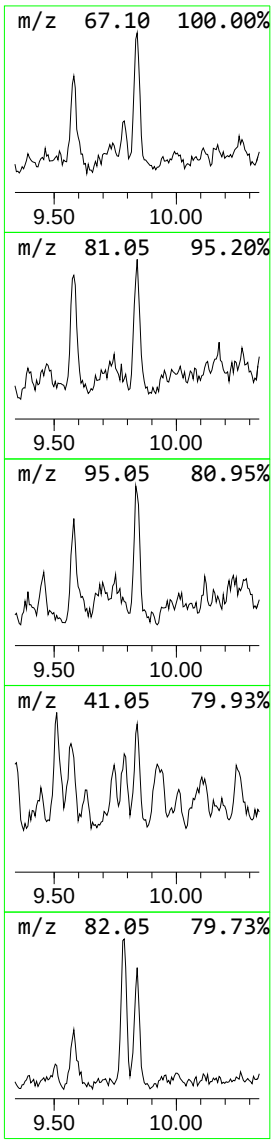
****
Peak Number 3 Decalin, syn-1-methyl-, cis- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.839	2.12 ng	259797	Naphthalene-d8	10.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	76
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	68
3	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	64
4	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	64
5	9-Octadecyne	250	C18H34	035365-59-4	64





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Instrument :
BNA_M
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365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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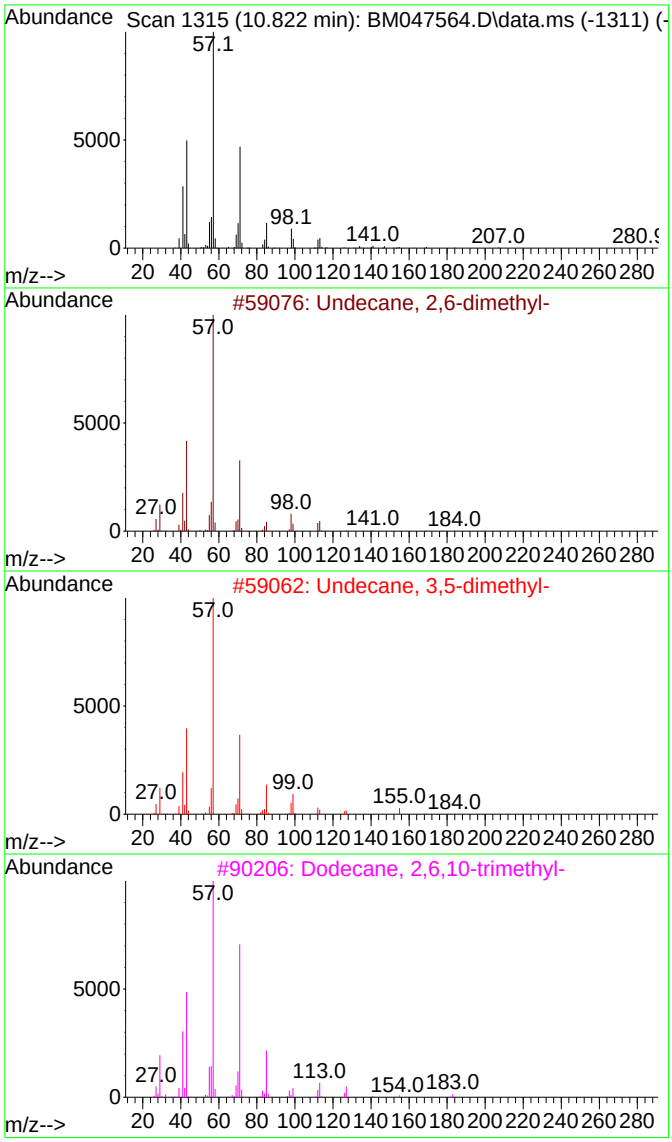
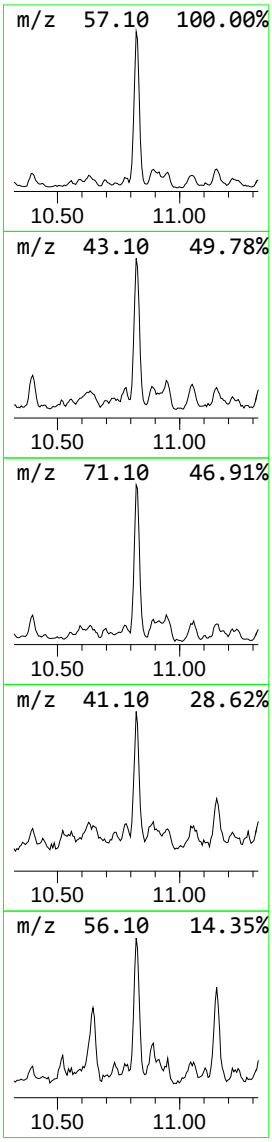
Peak Number 4 Undecane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	4.53 ng	554728	Naphthalene-d8	10.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	95
2	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	64
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
4	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	59
5	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	53





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Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
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TIC Library : C:\Database\NIST20.L
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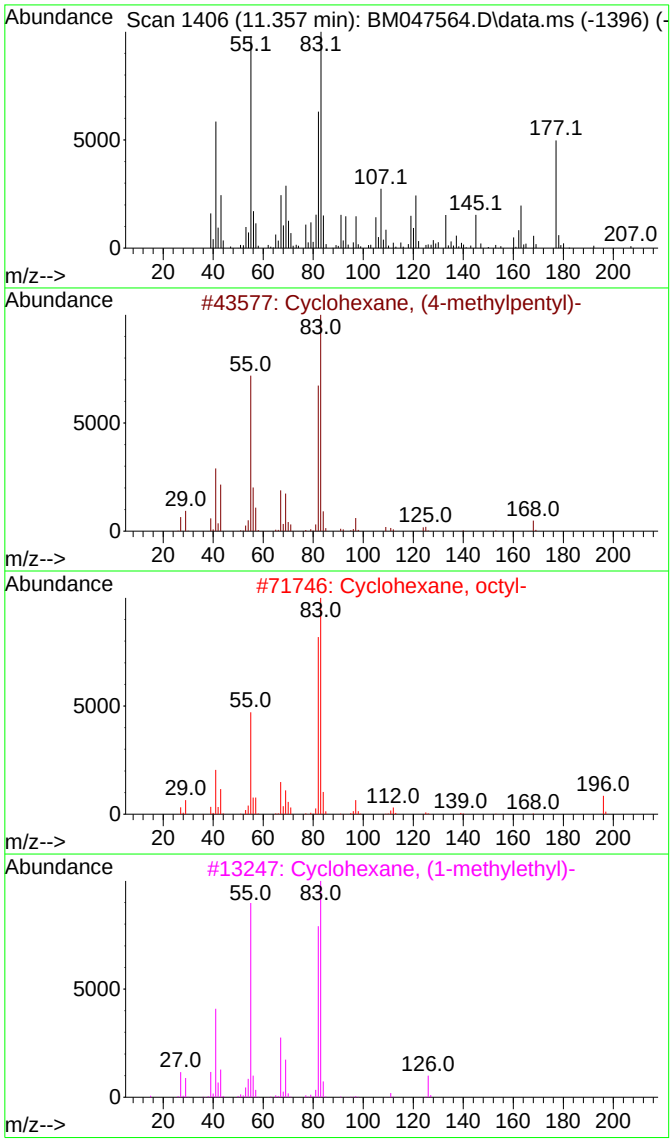
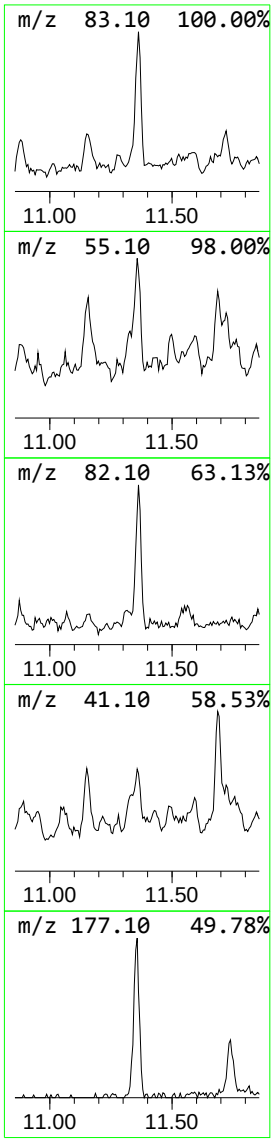
****

Peak Number 5 unknown11.357 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.357	3.83 ng	468562	Naphthalene-d8	10.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	43
2	Cyclohexane, octyl-	196	C14H28	001795-15-9	38
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38
4	Cyclohexane, pentyl-	154	C11H22	004292-92-6	38
5	Cyclohexane, decyl-	224	C16H32	001795-16-0	38





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BNA_M
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365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
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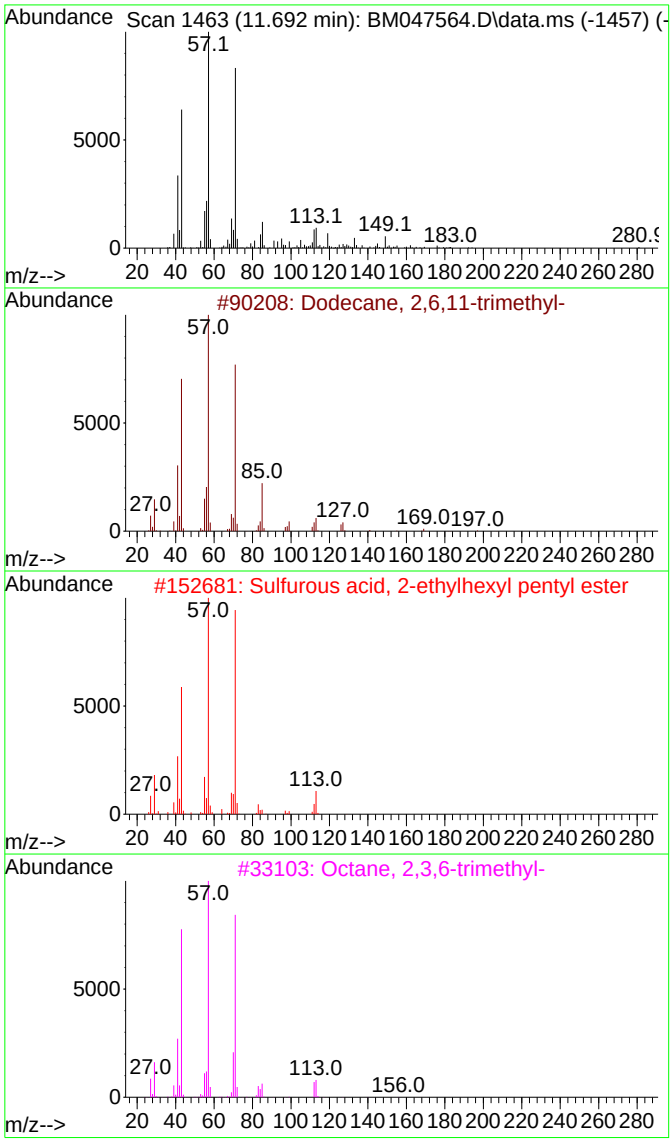
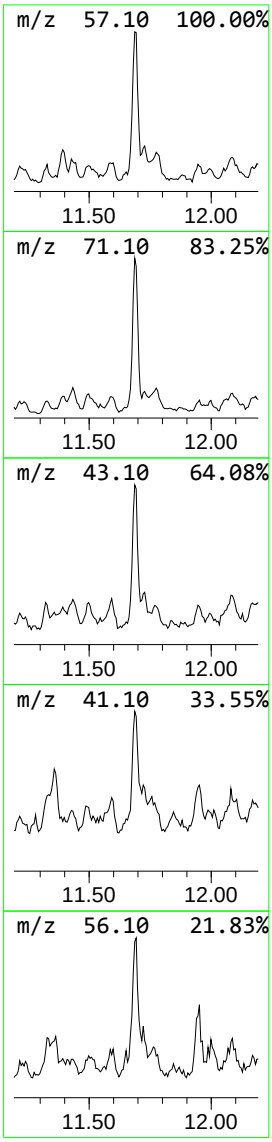
Peak Number 6 Dodecane, 2,6,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.692	4.44 ng	543822	Naphthalene-d8	10.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
2	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	59
3	Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	59
4	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	59
5	3-(Octyloxy)-1,2-propanediol	204	C11H24O3	010438-94-5	53





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Operator : RC/JU
Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
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365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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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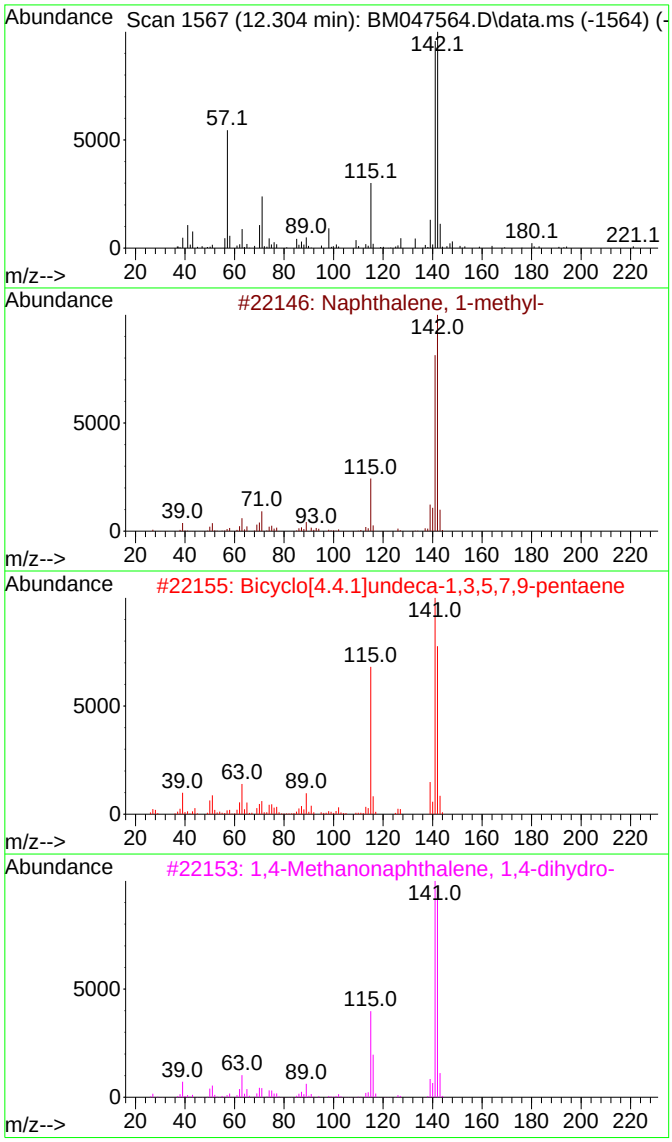
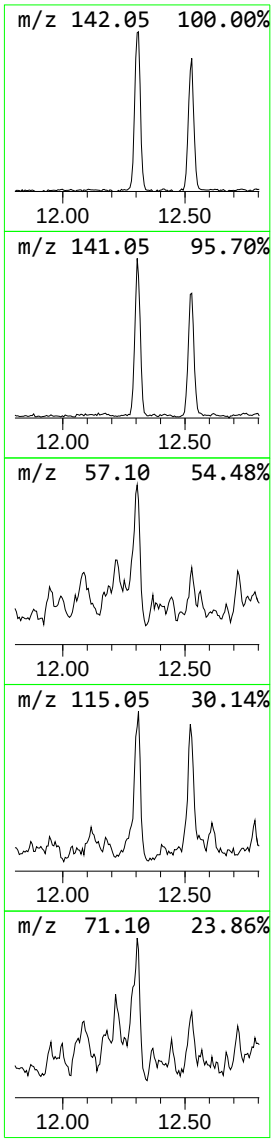
Peak Number 7 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	2.95 ng	360893	Naphthalene-d8	10.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
2	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	83
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	81
4	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	80
5	Benzocycloheptatriene	142	C11H10	000264-09-5	72





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TIC Library : C:\Database\NIST20.L
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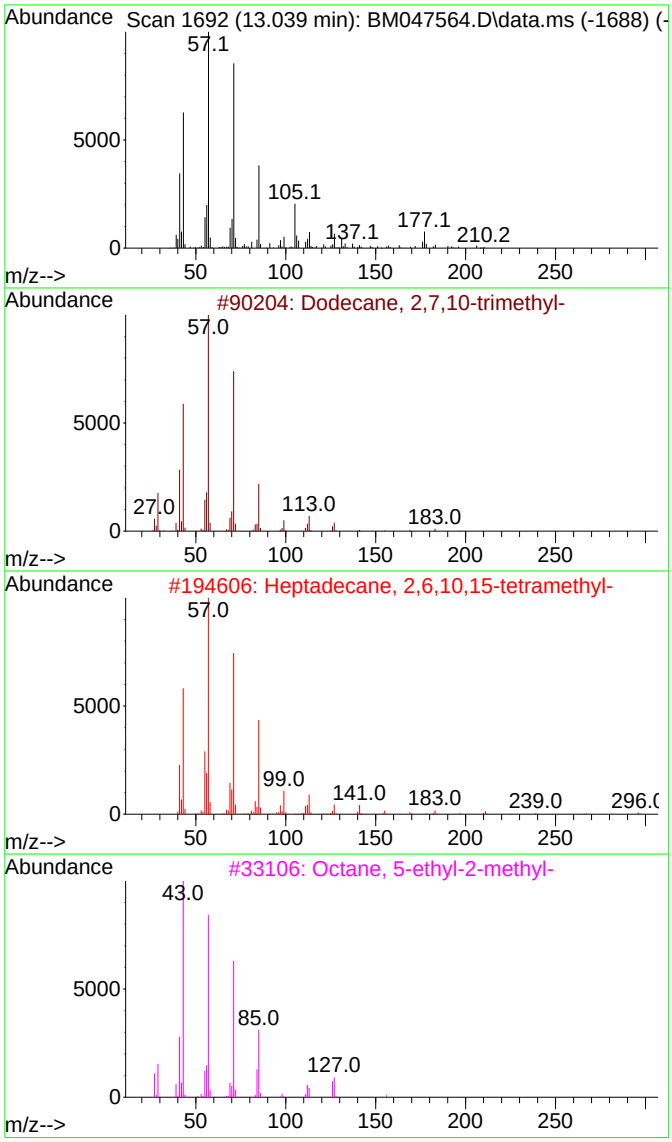
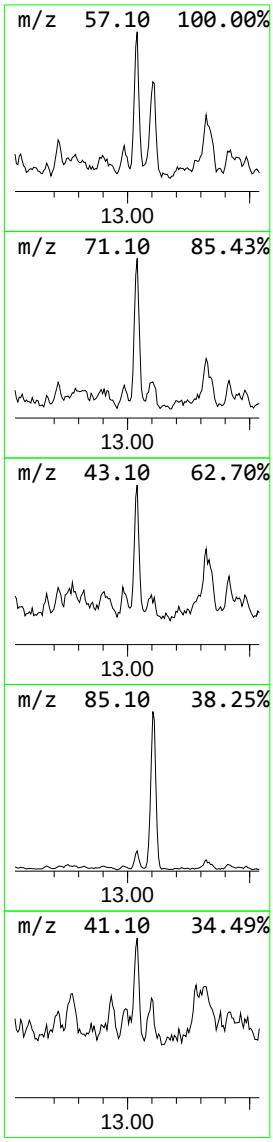
Peak Number 8 Dodecane, 2,7,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.039	2.29 ng	327096	Acenaphthene-d10	14.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
3	Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	59
4	Decane, 3-methyl-	156	C11H24	013151-34-3	58
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	52





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
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TIC Library : C:\Database\NIST20.L
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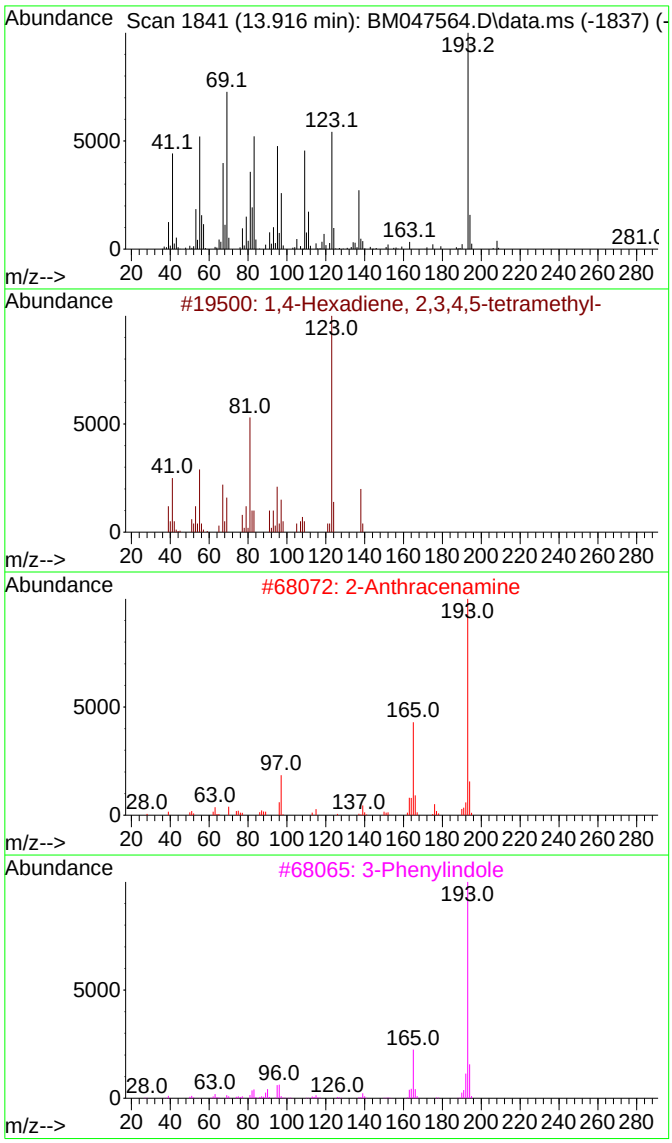
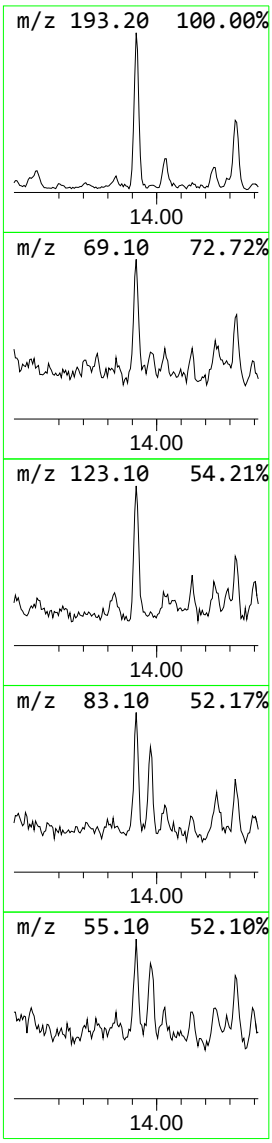
Peak Number 9 unknown13.916 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	2.02 ng	288143	Acenaphthene-d10	14.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	22
2	2-Anthracenamine	193	C14H11N	000613-13-8	18
3	3-Phenylindole	193	C14H11N	001504-16-1	18
4	2-Phenylindolizine	193	C14H11N	025379-20-8	14
5	3-((2R,5S)-7-(Cyclohexylsulfonyl...	340	C17H28N2O3S	1000483-82-6	14





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Acq On : 18 Sep 2024 20:25
Operator : RC/JU
Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
365-351-294

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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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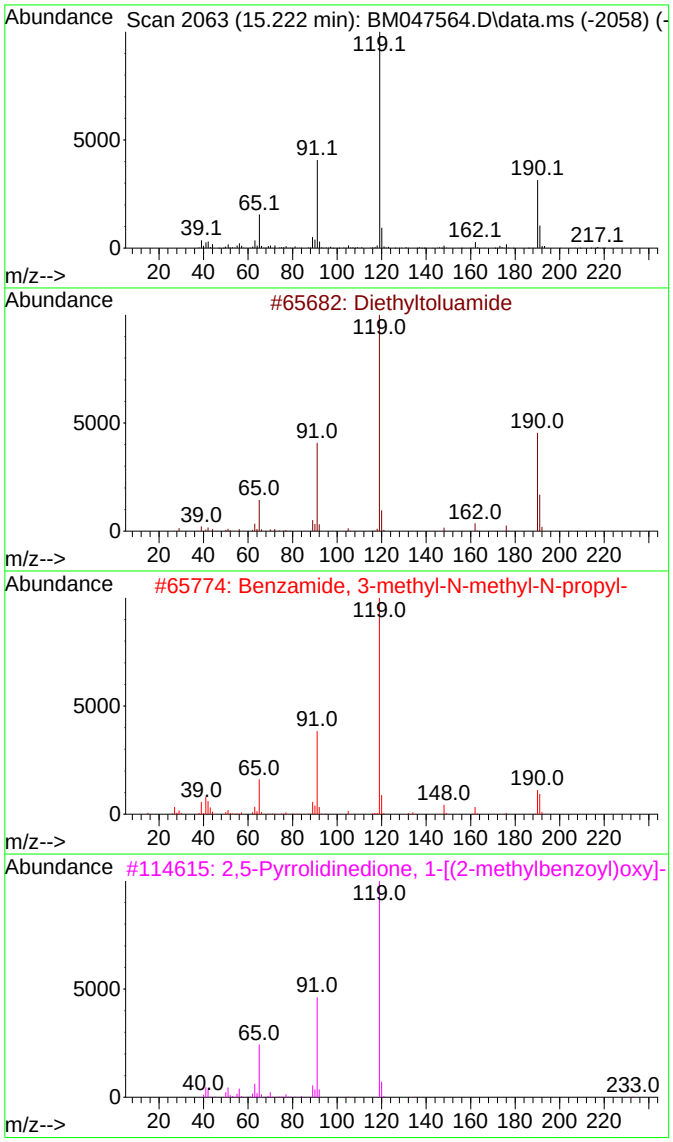
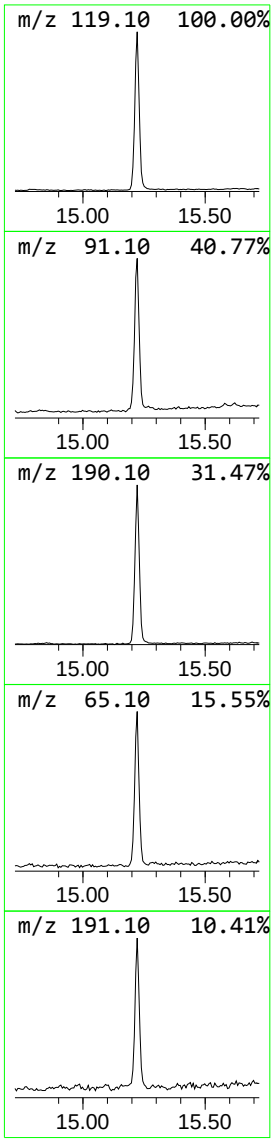
Peak Number 10 Diethyltoluamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.222	6.97 ng	994244	Acenaphthene-d10	14.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	97
2	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	93
3	2,5-Pyrrolidinedione, 1-[(2-meth...	233	C12H11NO4	110920-14-4	89
4	Benzamide, 2-methyl-N-methyl-N-p...	191	C12H17NO	1000421-44-4	87
5	Benzamide, 3-methyl-N-isobutyl-	191	C12H17NO	1000407-41-0	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047564.D
Acq On : 18 Sep 2024 20:25
Operator : RC/JU
Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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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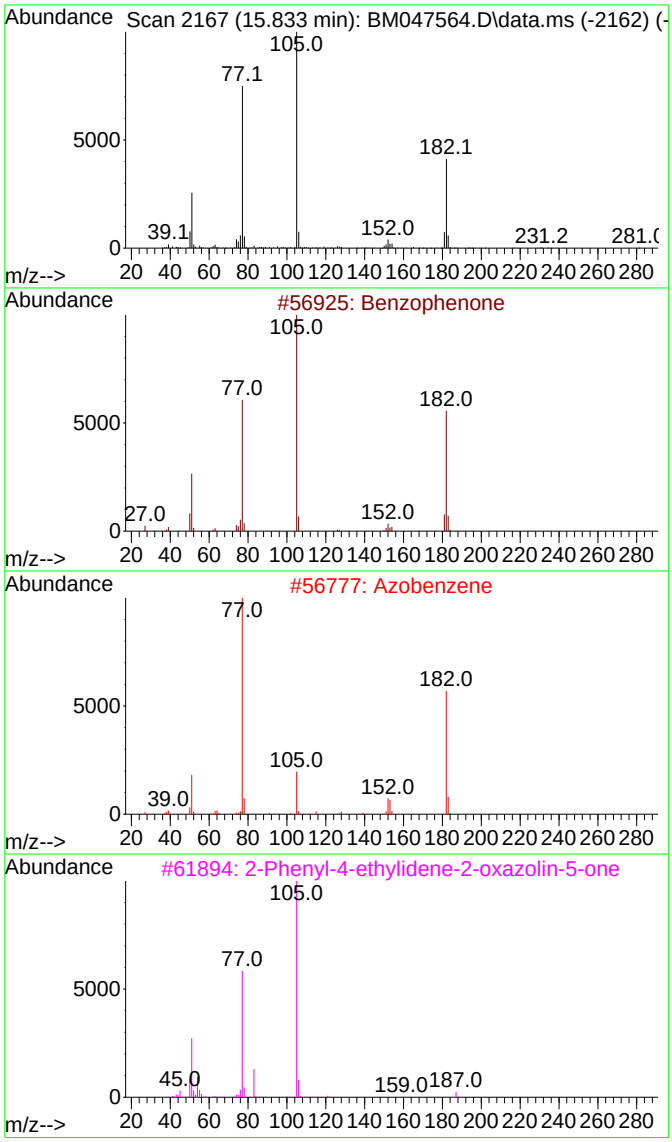
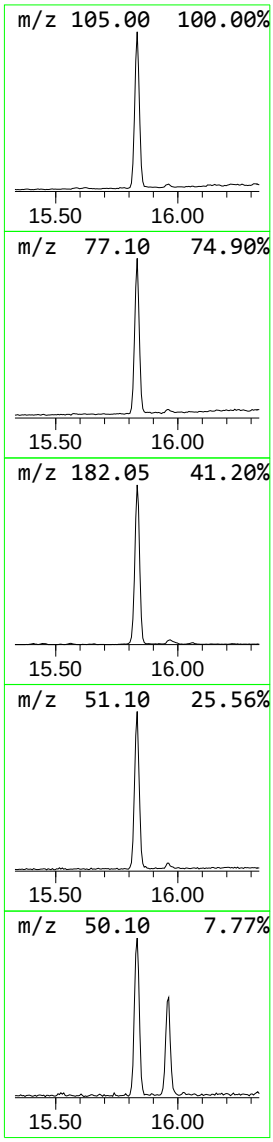
Peak Number 11 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.833	10.38 ng	1480490	Acenaphthene-d10	14.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	53
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	53
5	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091824\
Data File : BM047564.D
Acq On : 18 Sep 2024 20:25
Operator : RC/JU
Sample : P4089-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
365-351-294

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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-Pentanone, 4-...	4.963	3.5	ng	313877	1	7.851	1767880	20.0
Hexane, 3,3-dim...	9.510	2.0	ng	246724	2	10.645	2448460	20.0
Decalin, syn-1-...	9.839	2.1	ng	259797	2	10.645	2448460	20.0
Undecane, 2,6-d...	10.822	4.5	ng	554728	2	10.645	2448460	20.0
unknown11.357	11.357	3.8	ng	468562	2	10.645	2448460	20.0
Dodecane, 2,6,1...	11.692	4.4	ng	543822	2	10.645	2448460	20.0
Bicyclo[4.4.1]u...	12.304	3.0	ng	360893	2	10.645	2448460	20.0
Dodecane, 2,7,1...	13.039	2.3	ng	327096	3	14.480	2853850	20.0
unknown13.916	13.916	2.0	ng	288143	3	14.480	2853850	20.0
Diethyltoluamide	15.222	7.0	ng	994244	3	14.480	2853850	20.0
Benzophenone	15.833	10.4	ng	1480490	3	14.480	2853850	20.0