LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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: BF138404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	10	19	23	rVB	7328897	10967103	100.00%	24.544%
2	5.092	508	511	518	rVB	308175	355902	3.25%	0.796%
3	5.504	576	581	584	rBV	3225066	3040210	27.72%	6.804%
4	6.504	747	751	757	rVB	2283263	1917976	17.49%	4.292%
5	6.875	810	814	817	rBV	1399139	1196768	10.91%	2.678%
6	7.439	900	910	913	rBV	3762085	3956734	36.08%	8.855%
7	7.722	954	958	961	rVB	246913	184362	1.68%	0.413%
8	7.822	968	975	980	rBV2	137847	155406	1.42%	0.348%
9	8.157	1028	1032	1035	rVB	1679937	1510296	13.77%	3.380%
10	8.410	1070	1075	1080	rBV2	725048	710489	6.48%	1.590%
11	8.463	1080	1084	1088	rVB2	140653	168316	1.53%	0.377%
12	8.557	1094	1100	1106	rBV	405751	513176	4.68%	1.148%
13	8.745	1127	1132	1135	rBV	1426273	1118456	10.20%	2.503%
14	8.863	1146	1152	1154	rBV4	89399	109938	1.00%	0.246%
15	8.892	1154	1157	1159	rVB	158390	122015	1.11%	0.273%
16	8.963	1164	1169	1171	rBV	271559	265798	2.42%	0.595%
17	9.192	1205	1208	1210	rBV	141974	123410	1.13%	0.276%
18	9.233	1210	1215	1218	rVV	6042330	5801174	52.90%	12.983%
19	9.263	1218	1220	1226	rVB	146754	137420	1.25%	0.308%
20	9.392	1238	1242	1249	rBV	215609	209449	1.91%	0.469%
21	9.469	1249	1255	1257	rBV	190816	206746	1.89%	0.463%
22	9.492	1257	1259	1262	rVB	680965	484938	4.42%	1.085%
23	9.904	1326	1329	1333	rBV	1738198	1607899	14.66%	3.598%
24	10.004	1342	1346	1349	rBV2	110037	141555	1.29%	0.317%
25	10.698	1459	1464	1467	rBV	3346067	3044510	27.76%	6.814%
26	11.392	1578	1582	1585	rBV	1607805	1265962	11.54%	2.833%
27	11.916	1667	1671	1676	rBV	170684	184954	1.69%	0.414%
28	12.980	1847	1852	1855	rBV	3515016	3542848	32.30%	7.929%
29	14.027	2024	2030	2036	rBV	1004620	890932	8.12%	1.994%
30	15.492	2274	2279	2284	rBV	623469	748542	6.83%	1.675%

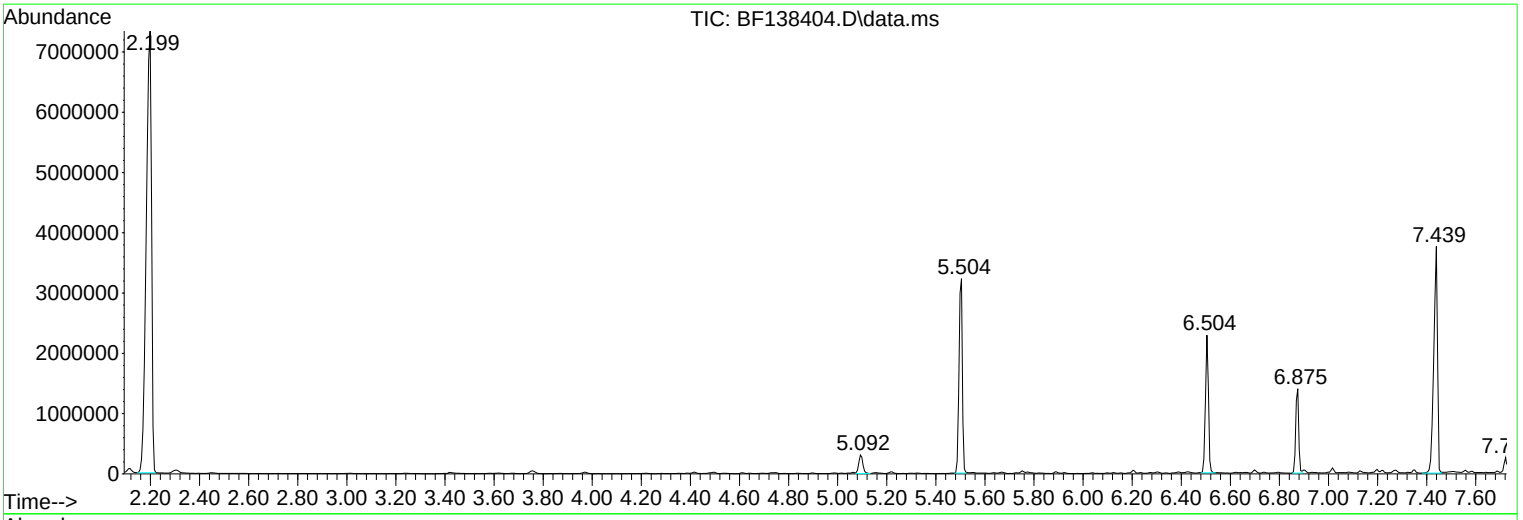
Sum of corrected areas: 44683284

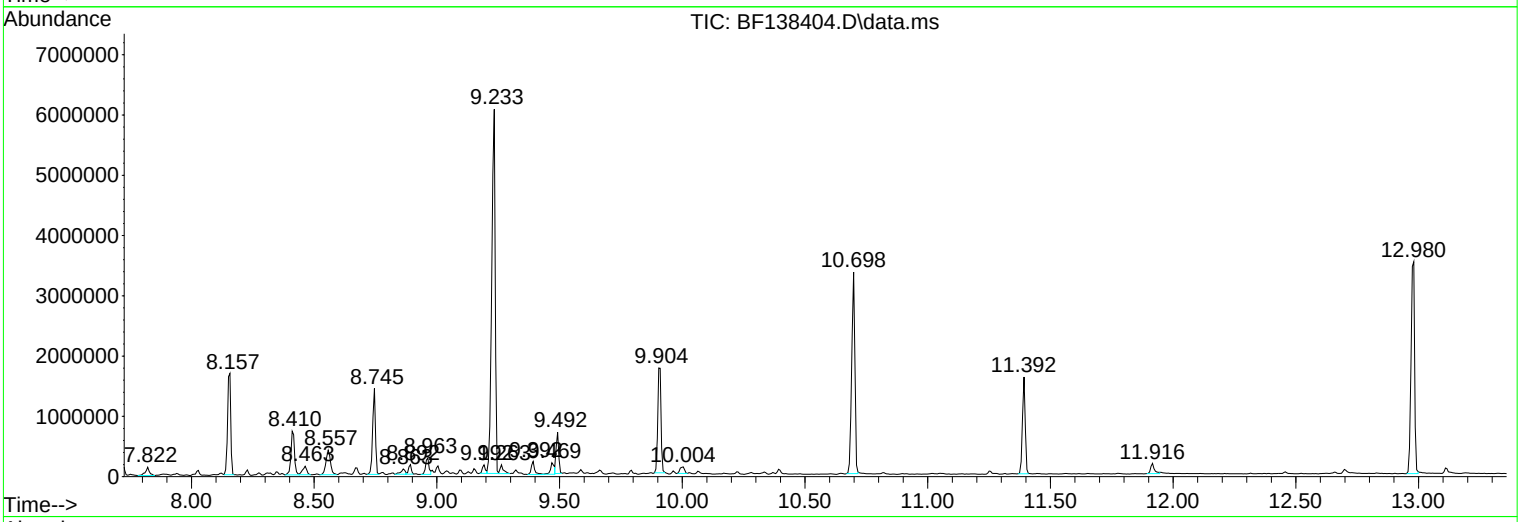
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

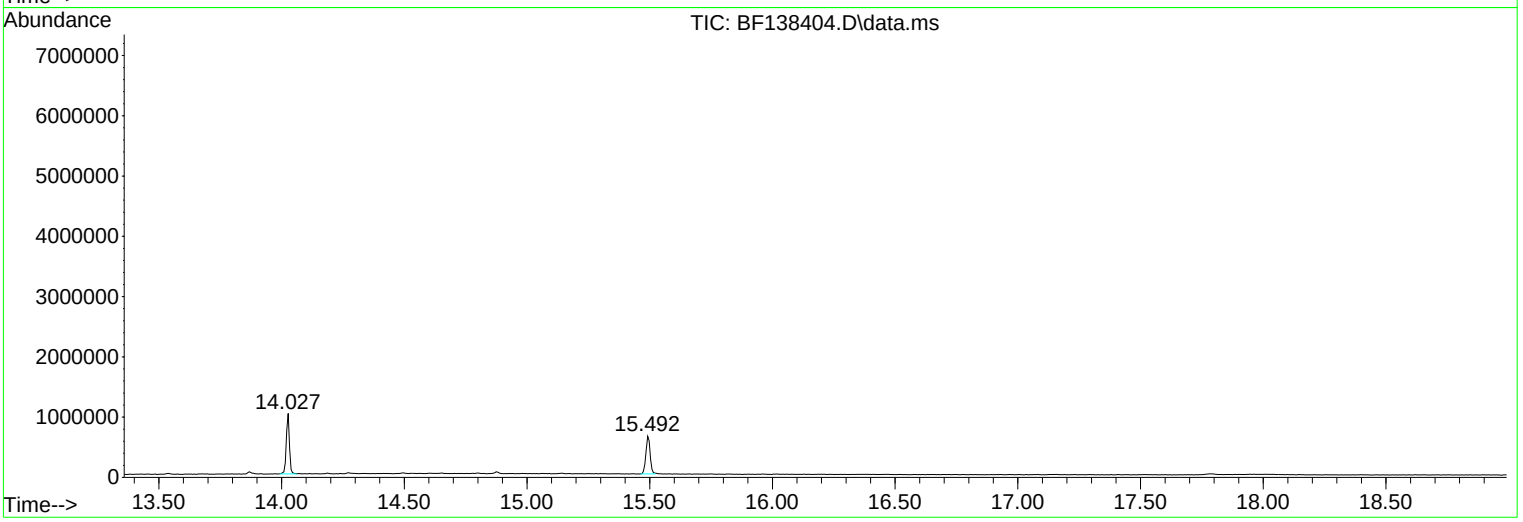
Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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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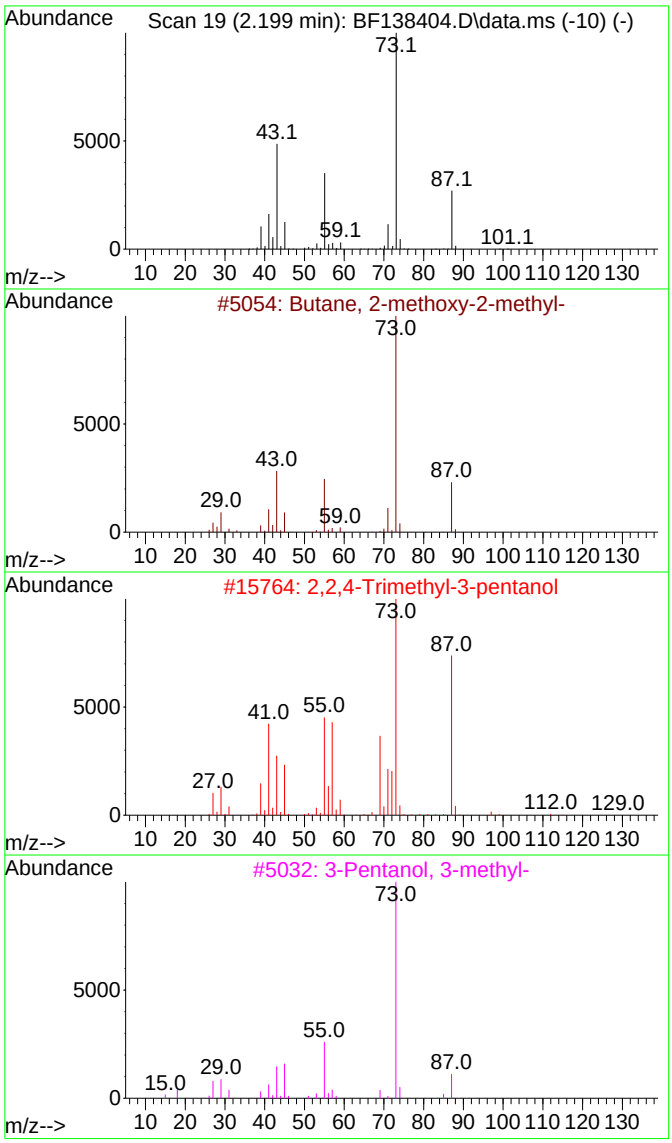
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

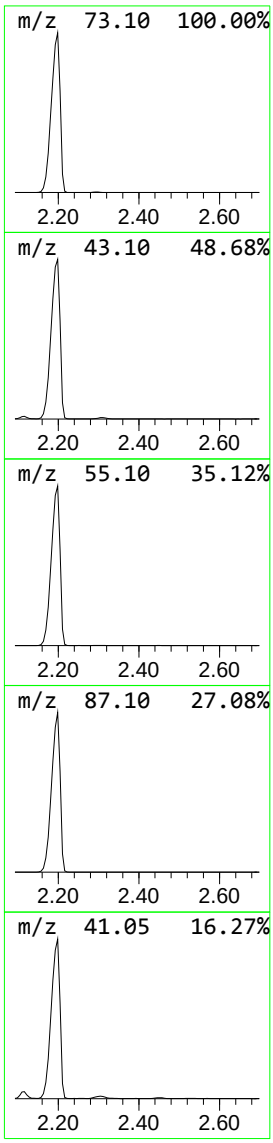
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	183.28 ng	10967100	1,4-Dichlorobenzene-d4	6.875

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	40
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF138404.D
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Operator : CG\JU
Sample : P3092-06
Misc :
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Instrument :
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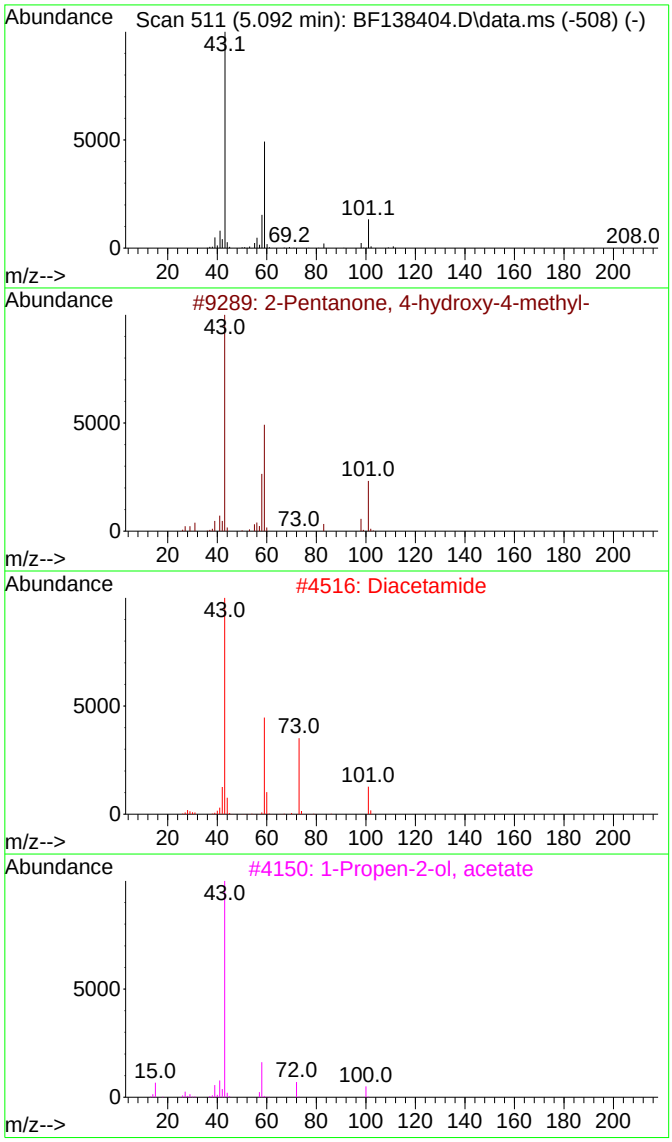
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

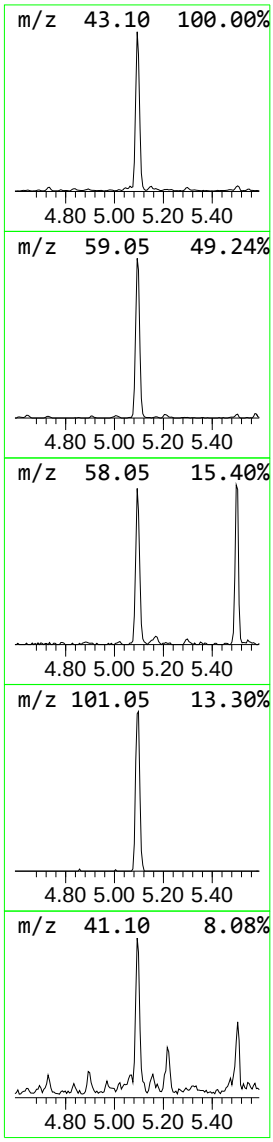
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	5.95 ng	355902	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Diacetamide	101	C4H7NO2	000625-77-4	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7





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Sample : P3092-06
Misc :
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Instrument :
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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

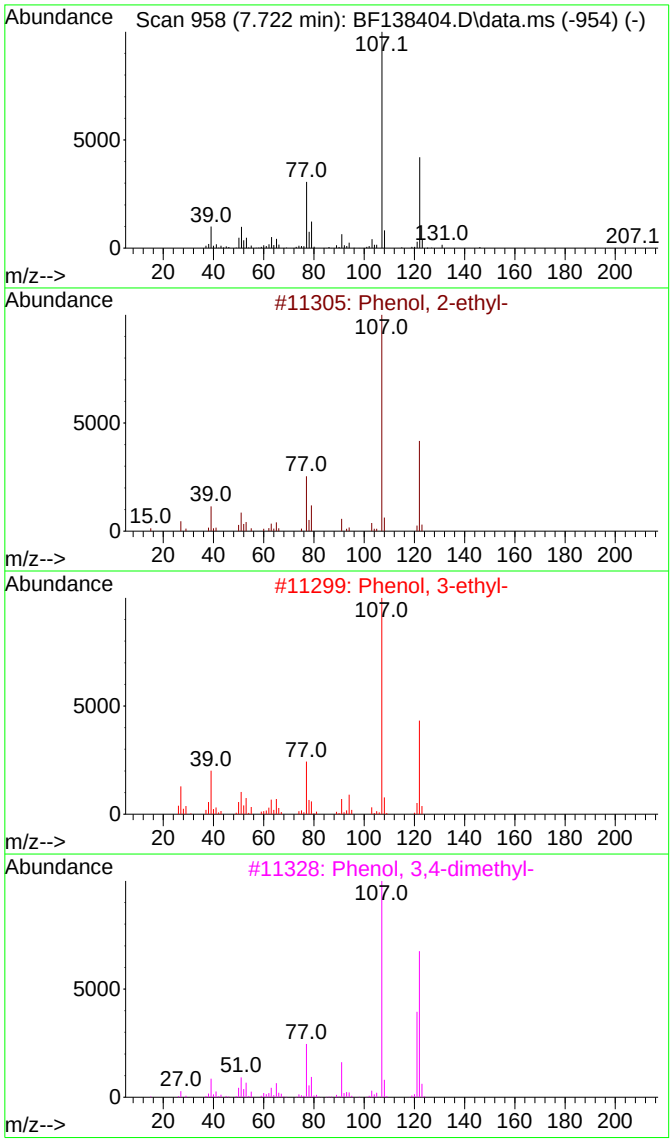
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

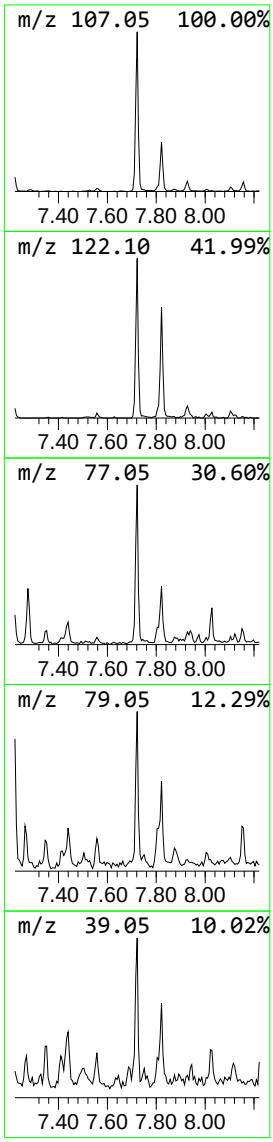
****

Peak Number 3 Phenol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	2.44 ng	184362	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-ethyl-	122	C8H10O	000090-00-6	95
2	Phenol, 3-ethyl-	122	C8H10O	000620-17-7	91
3	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	91
4	Phenol, 4-ethyl-	122	C8H10O	000123-07-9	87
5	Benzenemethanol, .alpha.-methyl-	122	C8H10O	000098-85-1	72





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Acq On : 01 Jul 2024 15:35
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Misc :
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BNA_F
ClientSampleId :
MW3-20240626

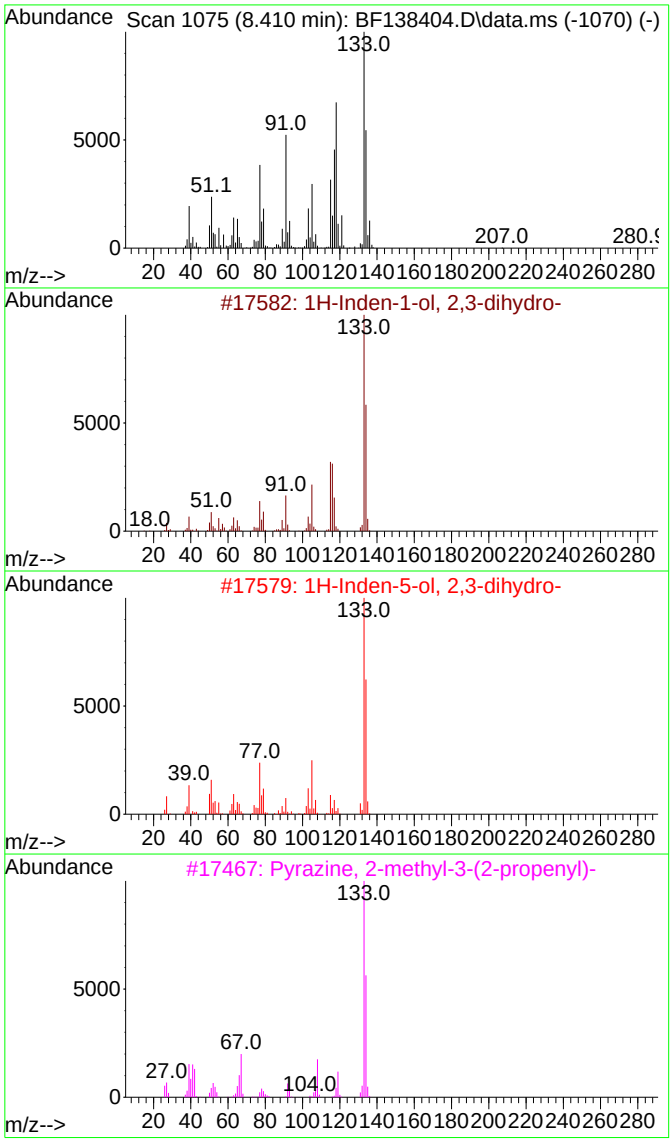
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

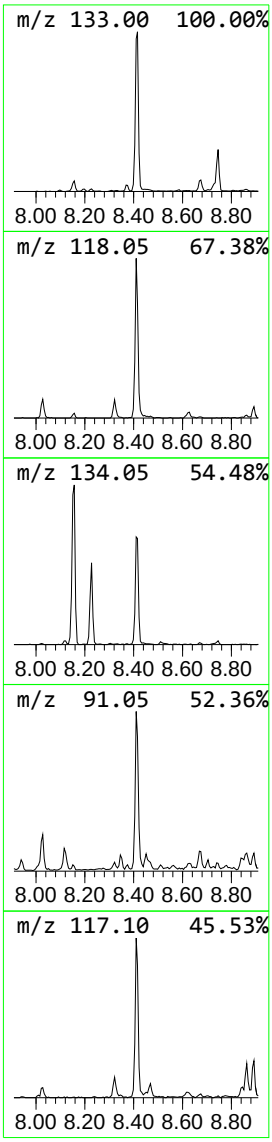
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-Inden-1-ol, 2,3-dihydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.410	9.41 ng	710489	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-ol, 2,3-dihydro-	134	C9H10O	006351-10-6	53
2	1H-Inden-5-ol, 2,3-dihydro-	134	C9H10O	001470-94-6	41
3	Pyrazine, 2-methyl-3-(2-propenyl)-	134	C8H10N2	055138-62-0	41
4	Benzaldehyde, 3,4-dimethyl-	134	C9H10O	005973-71-7	38
5	Tetrahydroquinoxaline	134	C8H10N2	003476-89-9	38





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Sample : P3092-06
Misc :
ALS Vial : 11 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

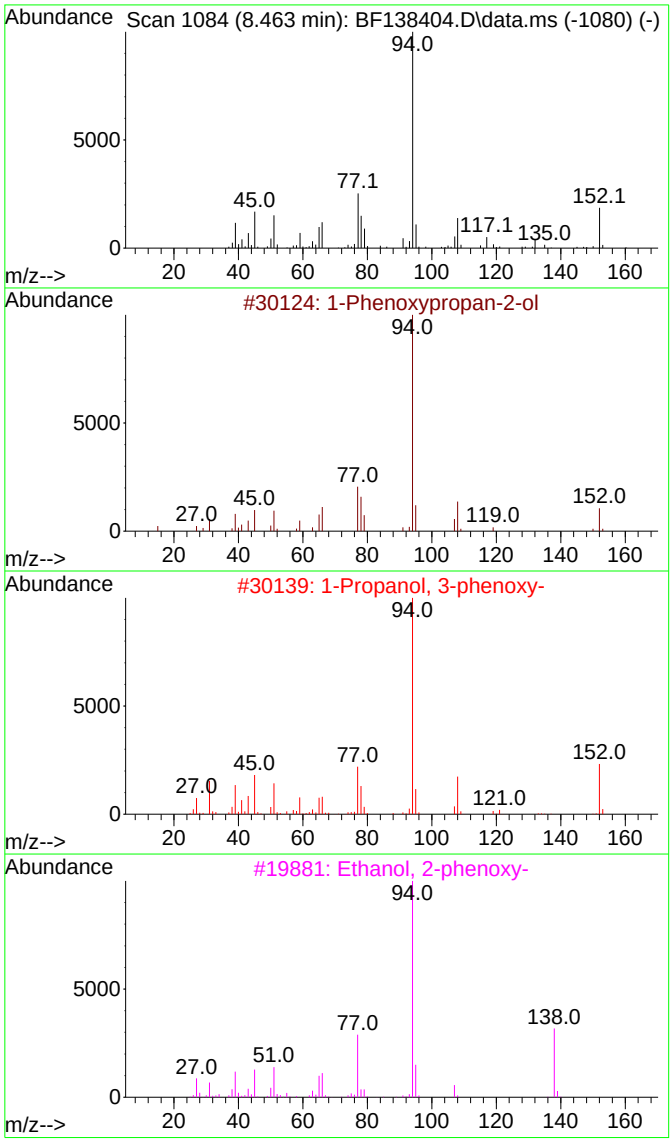
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

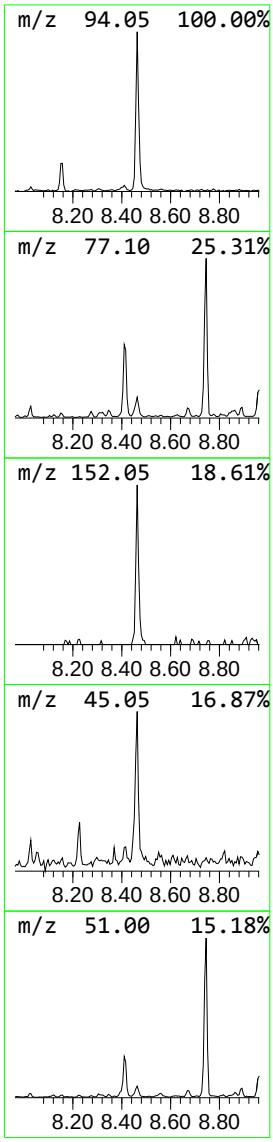
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.23 ng	168316	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53





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Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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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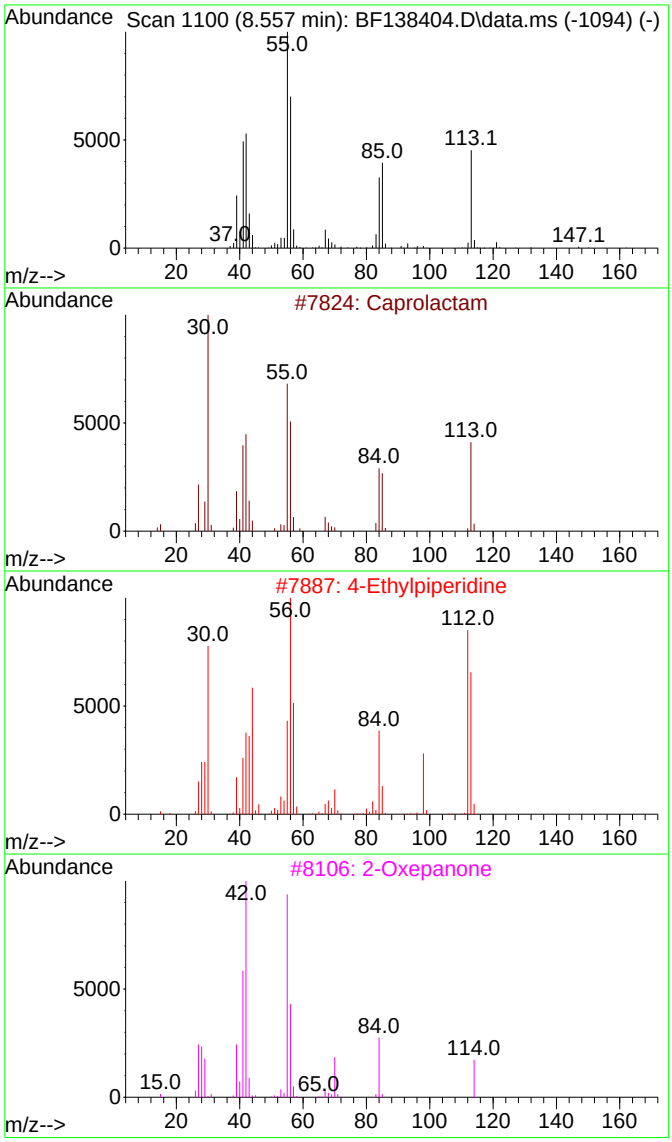
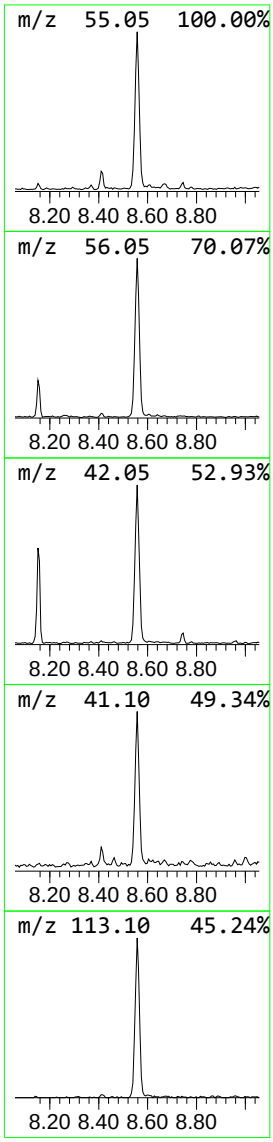
****

Peak Number 6 unknown8.557 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.557	6.80 ng	513176	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caprolactam	113	C6H11NO	000105-60-2	94
2	4-Ethylpiperidine	113	C7H15N	003230-23-7	47
3	2-Oxepanone	114	C6H10O2	000502-44-3	47
4	3,3-Dimethylpyrrolidin-2-one	113	C6H11NO	004831-43-0	46
5	1-Hexene	84	C6H12	000592-41-6	43





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Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 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

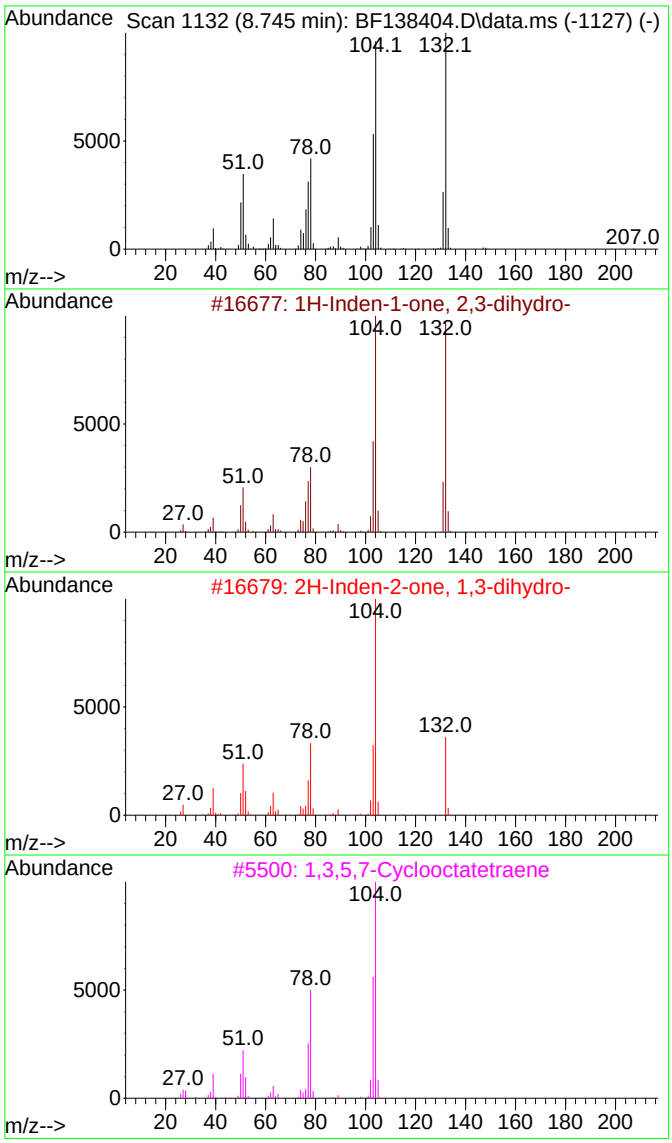
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

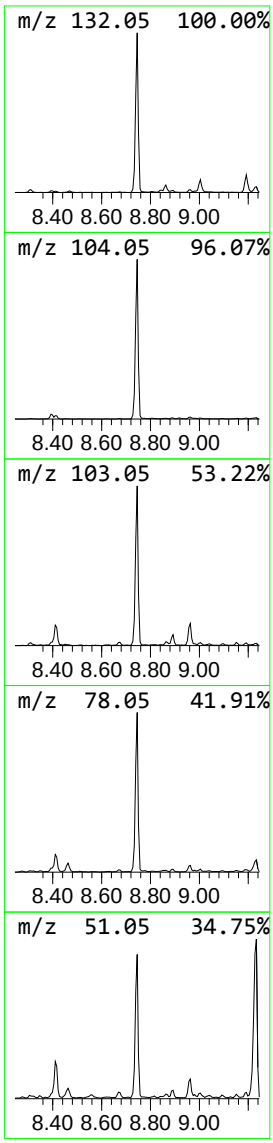
****

Peak Number 7 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.745	14.81 ng	1118460	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	96
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	64
3	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	64
4	Styrene	104	C8H8	000100-42-5	64
5	1H-Indenol	132	C9H8O	056631-57-3	60





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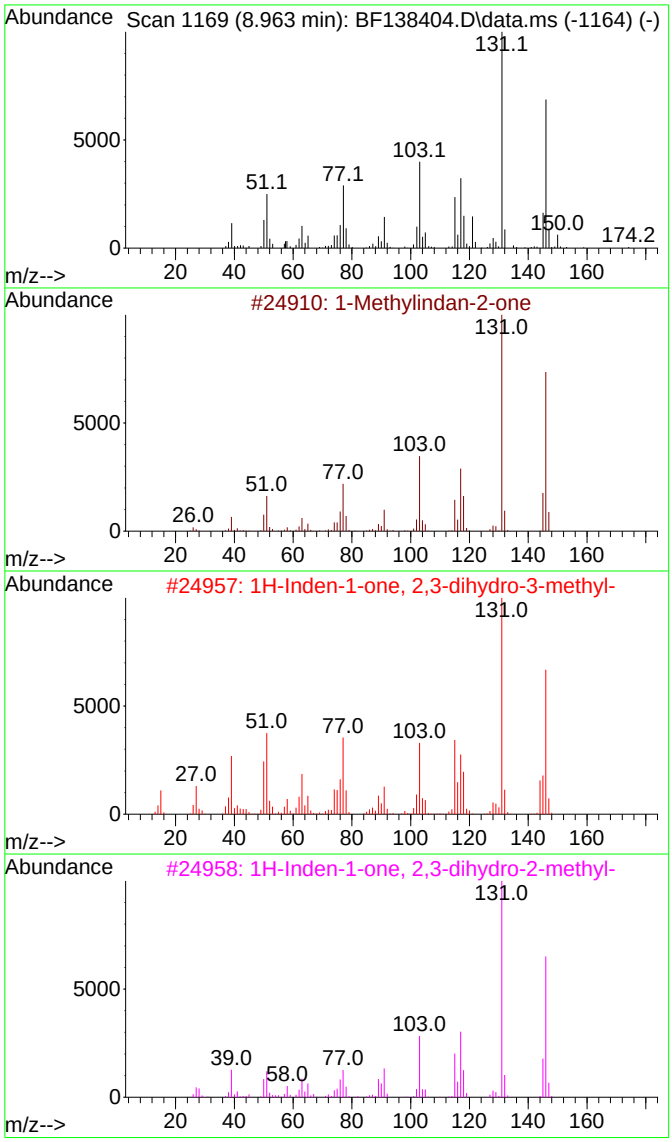
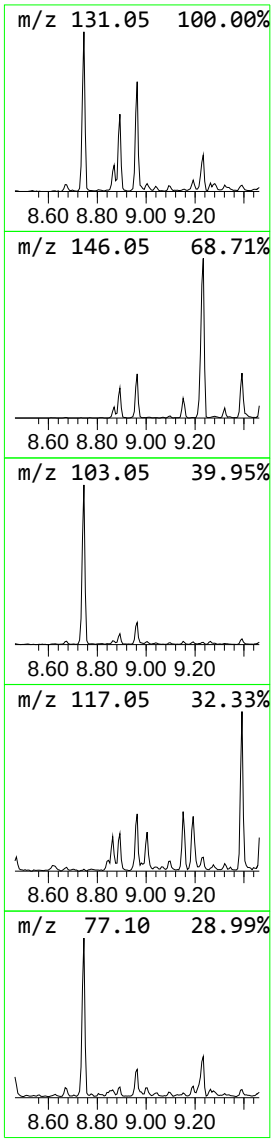
****

Peak Number 8 1-Methylindan-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.963	3.52 ng	265798	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methylindan-2-one	146	C10H10O	035587-60-1	96
2	1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	91
3	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	89
4	1-Decen-3-one, 5-hydroxy-4-penty...	316	C21H32O2	959035-43-9	59
5	1-Phenyldodec-1-en-3-one	258	C18H26O	872268-56-9	53





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Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 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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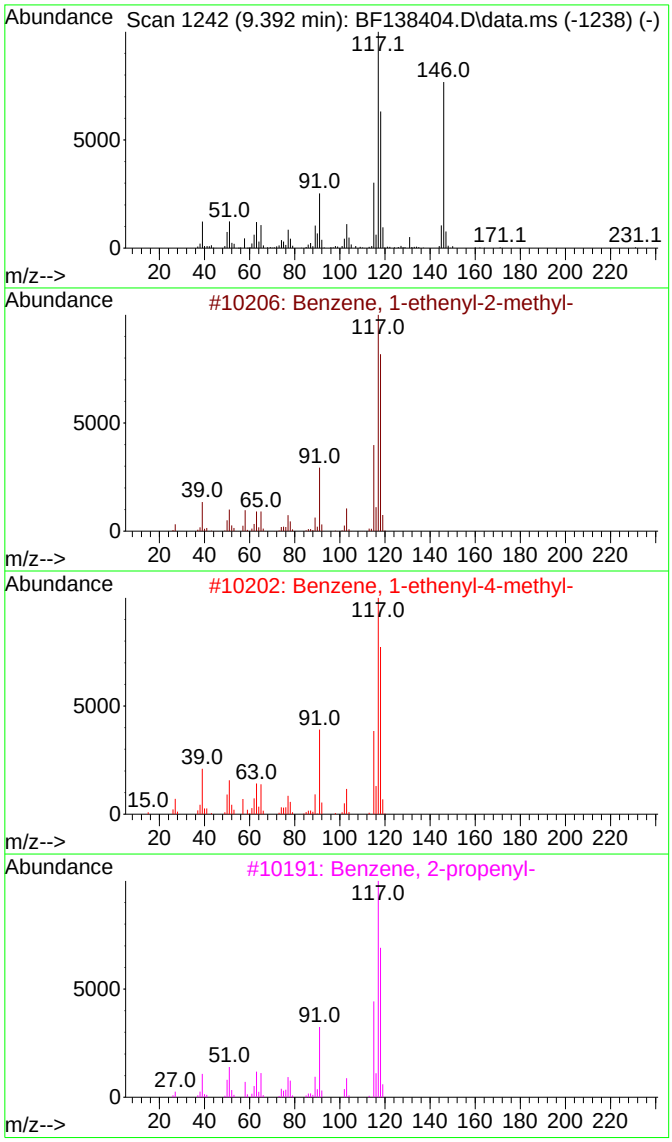
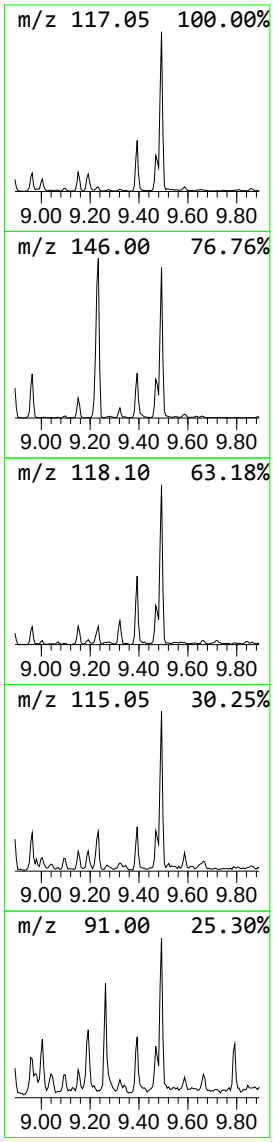
****

Peak Number 9 Benzene, 1-ethenyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.392	2.61 ng	209449	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
2	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	70
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	70
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64





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Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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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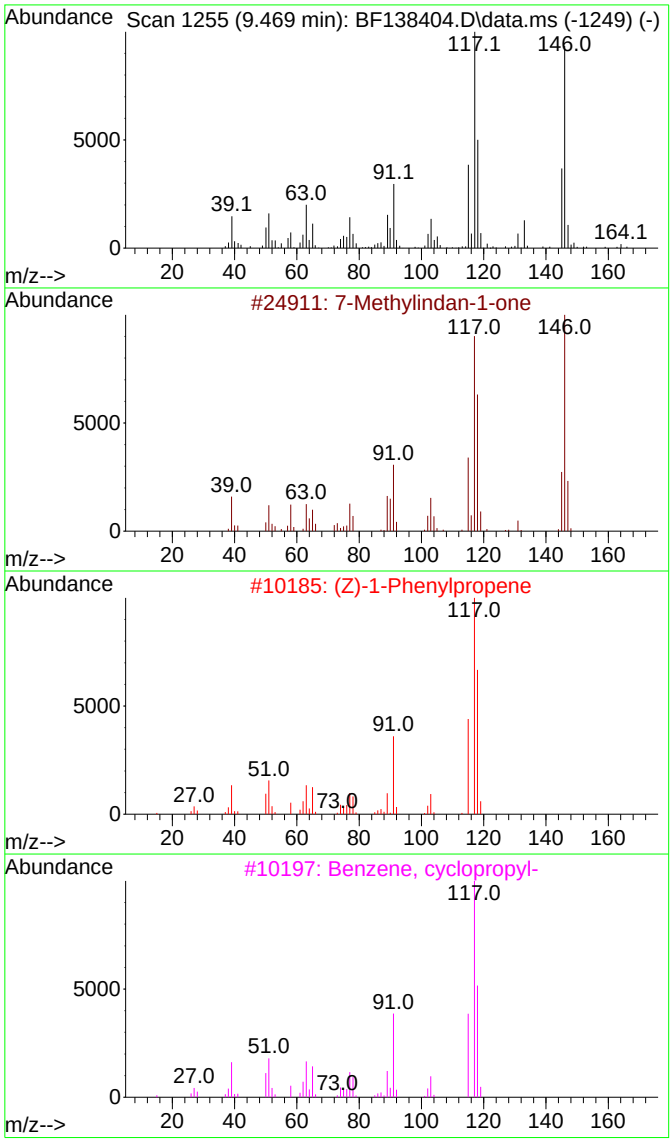
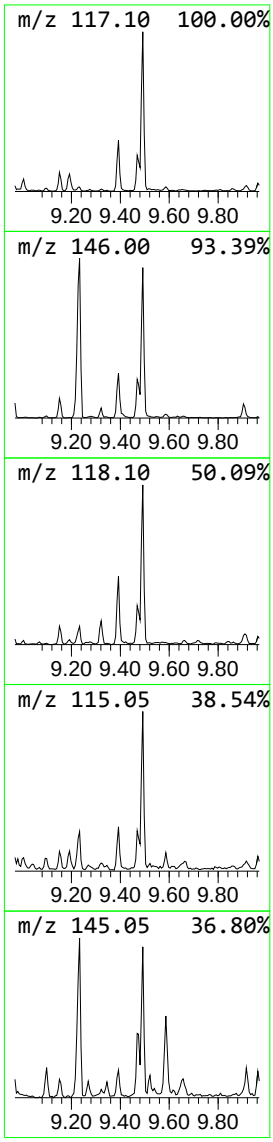
Peak Number 10 7-Methylindan-1-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.469	2.57 ng	206746	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methylindan-1-one	146	C10H10O	039627-61-7	90
2	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	86
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
4	1H-Imidazole, 4,5-dihydro-2-phenyl-	146	C9H10N2	000936-49-2	58
5	2(1H)-Quinazolinone	146	C8H6N2O	007471-58-1	50





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Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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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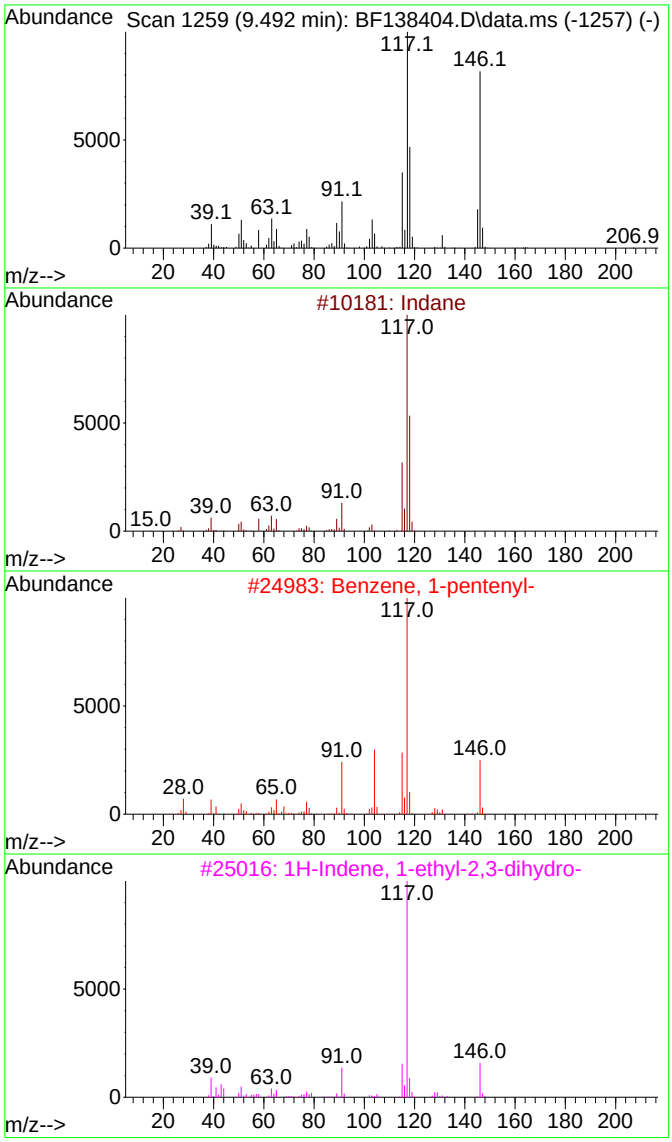
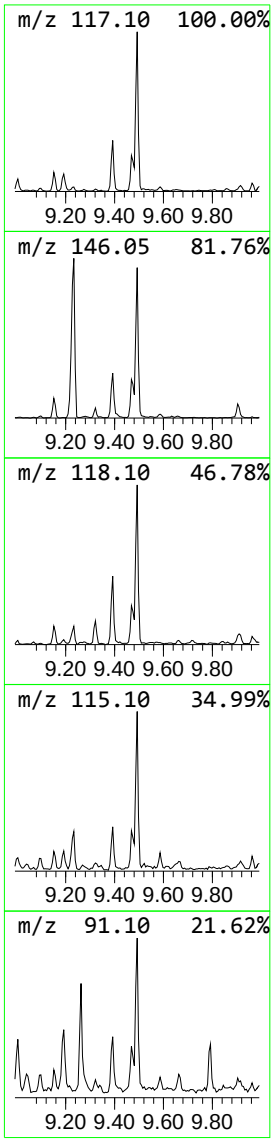
Peak Number 11 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	6.03 ng	484938	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	89
2	Benzene, 1-pentenyl-	146	C11H14	000826-18-6	68
3	1H-Indene, 1-ethyl-2,3-dihydro-	146	C11H14	004830-99-3	58
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	51
5	Deltacyclene	118	C9H10	007785-10-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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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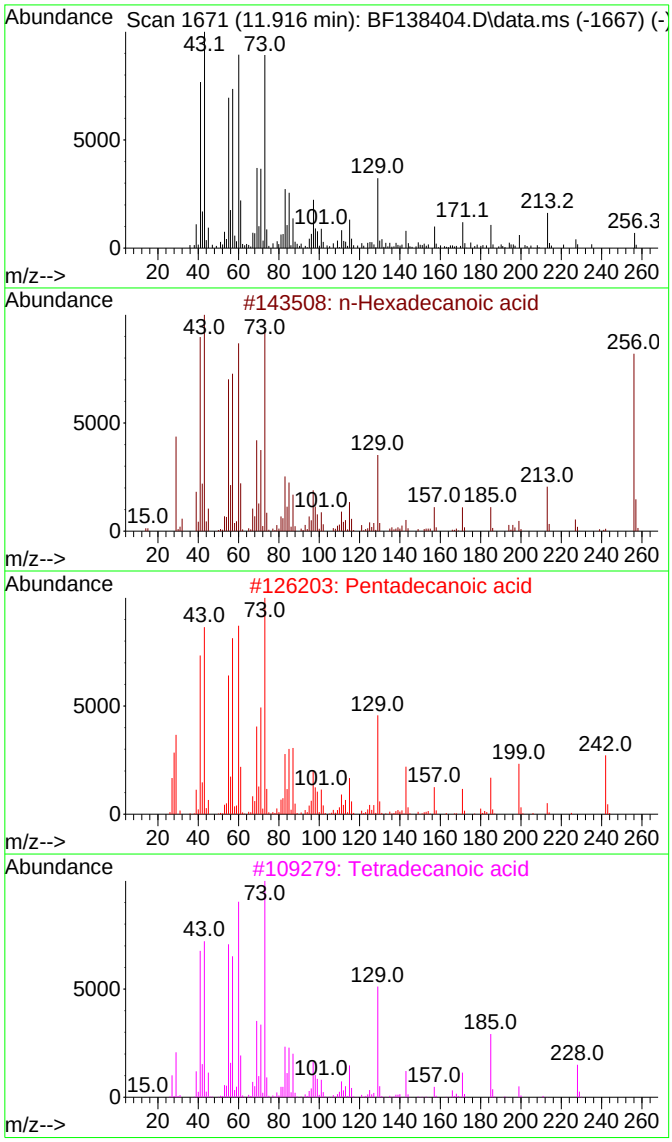
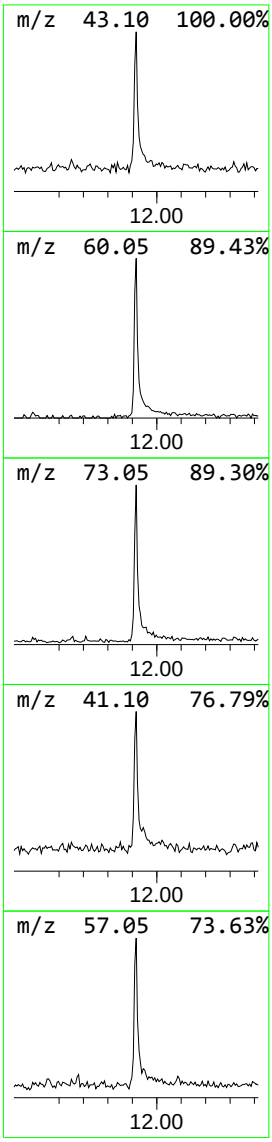
Peak Number 12 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.92 ng	184954	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138404.D
Acq On : 01 Jul 2024 15:35
Operator : CG\JU
Sample : P3092-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW3-20240626

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...	2.199	183.3	ng	10967100	1	6.875	1196770	20.0
2-Pentanone, 4-...	5.092	6.0	ng	355902	1	6.875	1196770	20.0
Phenol, 2-ethyl-	7.722	2.4	ng	184362	2	8.157	1510300	20.0
1H-Inden-1-ol, ...	8.410	9.4	ng	710489	2	8.157	1510300	20.0
1-Phenoxypropan...	8.463	2.2	ng	168316	2	8.157	1510300	20.0
unknown8.557	8.557	6.8	ng	513176	2	8.157	1510300	20.0
1H-Inden-1-one,...	8.745	14.8	ng	1118460	2	8.157	1510300	20.0
1-Methylindan-2...	8.963	3.5	ng	265798	2	8.157	1510300	20.0
Benzene, 1-ethe...	9.392	2.6	ng	209449	3	9.910	1607900	20.0
7-Methylindan-1...	9.469	2.6	ng	206746	3	9.910	1607900	20.0
Indane	9.492	6.0	ng	484938	3	9.910	1607900	20.0
n-Hexadecanoic ...	11.916	2.9	ng	184954	4	11.392	1265960	20.0