LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	14	23	rVB	1757445	2230842	96.25%	12.224%
2	3.405	222	224	238	rBV	9383	26446	1.14%	0.145%
3	4.463	401	404	409	rVB	41734	45270	1.95%	0.248%
4	5.093	505	511	514	rVB	1294399	1537745	66.34%	8.426%
5	5.493	575	579	582	rBV	1757888	1499040	64.67%	8.214%
6	6.498	745	750	753	rBV	1887085	1692071	73.00%	9.272%
7	6.863	808	812	815	rBV	669821	514073	22.18%	2.817%
8	7.428	899	908	911	rBV	1397710	1307894	56.43%	7.166%
9	7.675	947	950	955	rVB	29502	26326	1.14%	0.144%
10	8.145	1026	1030	1033	rVB	807006	673157	29.04%	3.689%
11	8.451	1079	1082	1088	rBV	48400	49055	2.12%	0.269%
12	9.222	1207	1213	1216	rBV	2465833	2317853	100.00%	12.700%
13	9.334	1228	1232	1236	rBV	182380	173233	7.47%	0.949%
14	9.822	1309	1315	1320	rBV	88772	75116	3.24%	0.412%
15	9.898	1324	1328	1331	rVV	909599	715573	30.87%	3.921%
16	9.992	1340	1344	1349	rVB	56144	69568	3.00%	0.381%
17	10.057	1349	1355	1357	rBV3	16187	24170	1.04%	0.132%
18	10.145	1367	1370	1373	rBV3	25422	25484	1.10%	0.140%
19	10.298	1393	1396	1398	rBV	25960	29855	1.29%	0.164%
20	10.322	1398	1400	1403	rVB	130730	94046	4.06%	0.515%
21	10.539	1432	1437	1440	rBV	40708	57381	2.48%	0.314%
22	10.686	1458	1462	1465	rBV	887062	781546	33.72%	4.282%
23	10.792	1477	1480	1485	rBV	126472	155034	6.69%	0.849%
24	11.245	1554	1557	1559	rBV	104746	86446	3.73%	0.474%
25	11.275	1559	1562	1568	rVB	57755	63827	2.75%	0.350%
26	11.380	1577	1580	1583	rBV	710185	613572	26.47%	3.362%
27	11.404	1583	1584	1589	rVB	73745	51539	2.22%	0.282%
28	11.622	1618	1621	1624	rBV3	20301	25119	1.08%	0.138%
29	11.669	1627	1629	1632	rVB	81875	60215	2.60%	0.330%
30	11.904	1666	1669	1672	rBV4	26073	28455	1.23%	0.156%
31	12.075	1696	1698	1701	rBV	45825	37125	1.60%	0.203%
32	12.592	1783	1786	1791	rVB	97278	90540	3.91%	0.496%
33	12.822	1820	1825	1829	rBV	70737	81110	3.50%	0.444%
34	12.886	1834	1836	1840	rVB3	26844	24199	1.04%	0.133%
35	12.963	1845	1849	1853	rBV	1658266	1493021	64.41%	8.181%
36	13.033	1858	1861	1866	rBV7	12785	24628	1.06%	0.135%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.533	1943	1946	1949	rVB	31108	26349	1.14%	0.144%
38	13.863	1999	2002	2018	rVB2	92969	165151	7.13%	0.905%
39	14.016	2024	2028	2031	rBV	494317	467477	20.17%	2.561%
40	14.039	2031	2032	2038	rVB	41965	37612	1.62%	0.206%
41	14.174	2052	2055	2059	rBV	29857	29366	1.27%	0.161%
42	14.480	2105	2107	2110	rBV	34582	29704	1.28%	0.163%
43	15.057	2201	2205	2208	rBV	35771	55420	2.39%	0.304%
44	15.121	2213	2216	2220	rBV3	23780	30895	1.33%	0.169%
45	15.357	2254	2256	2262	rVB	25176	28756	1.24%	0.158%
46	15.416	2263	2266	2272	rVB	21948	32795	1.41%	0.180%
47	15.480	2272	2277	2286	rBV	302377	401856	17.34%	2.202%
48	16.462	2437	2444	2453	rVB3	55679	112371	4.85%	0.616%
49	16.986	2529	2533	2539	rVB4	16467	31817	1.37%	0.174%

Sum of corrected areas: 18250143

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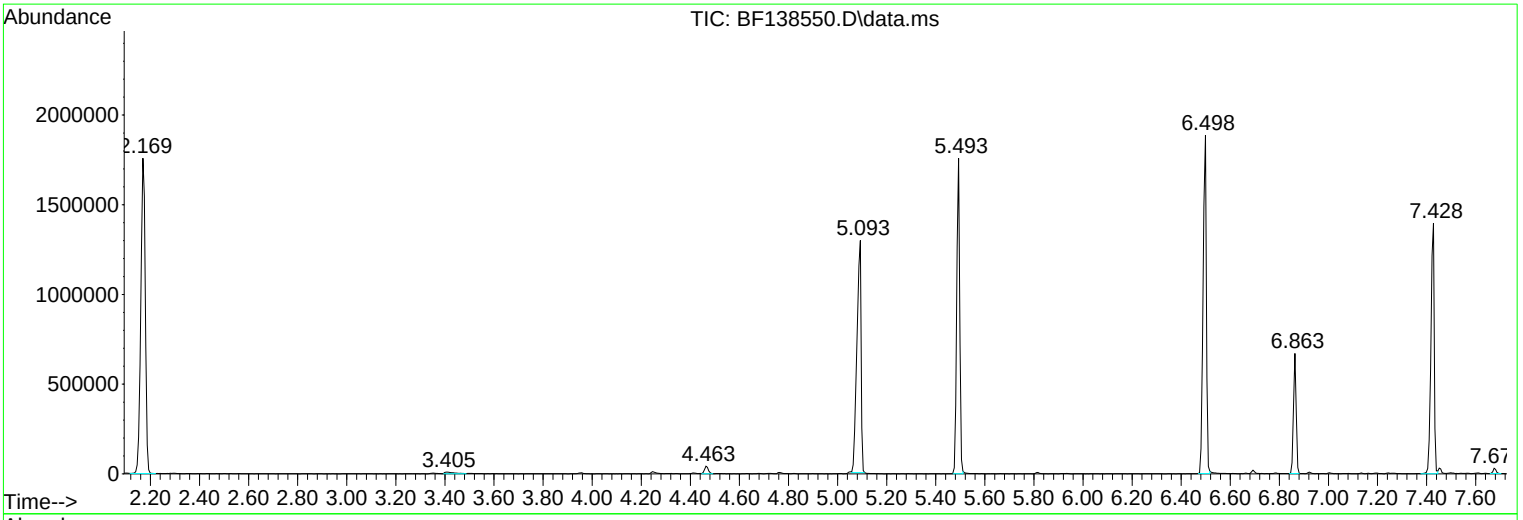
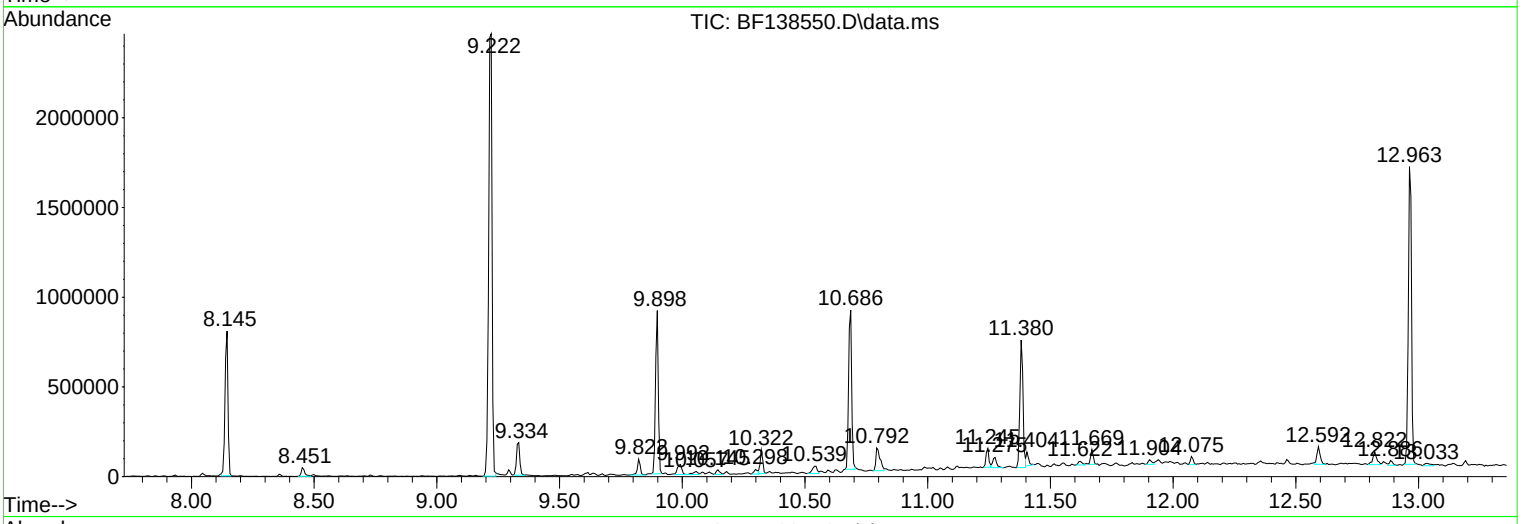
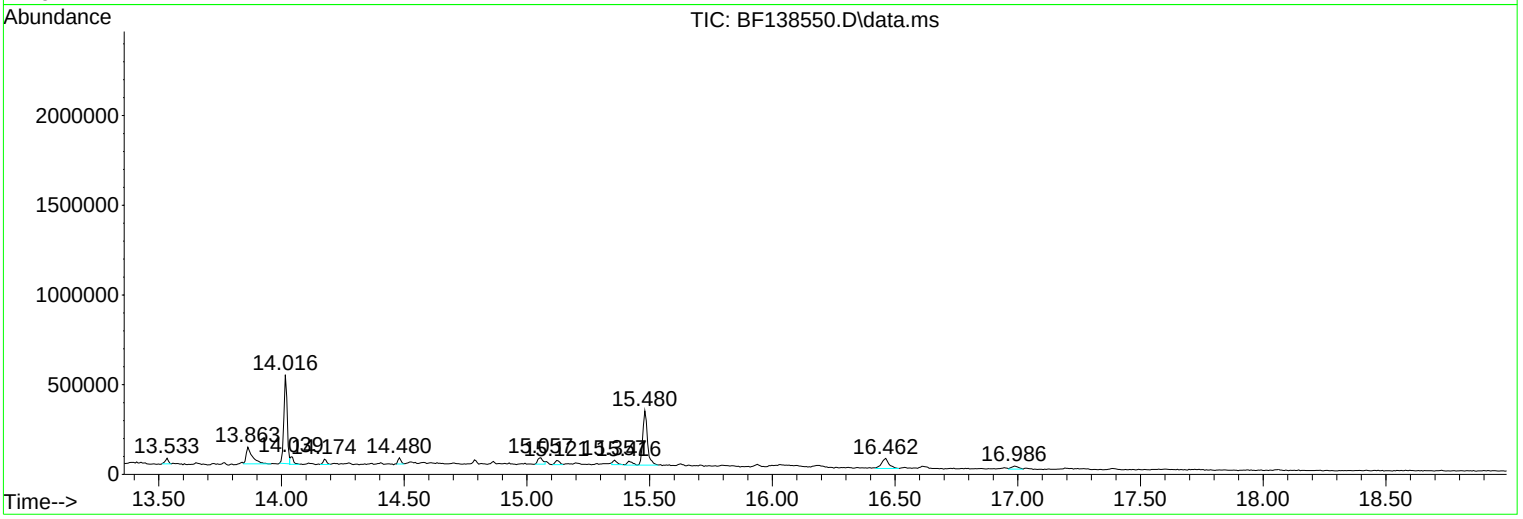
Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
CONC-PADS

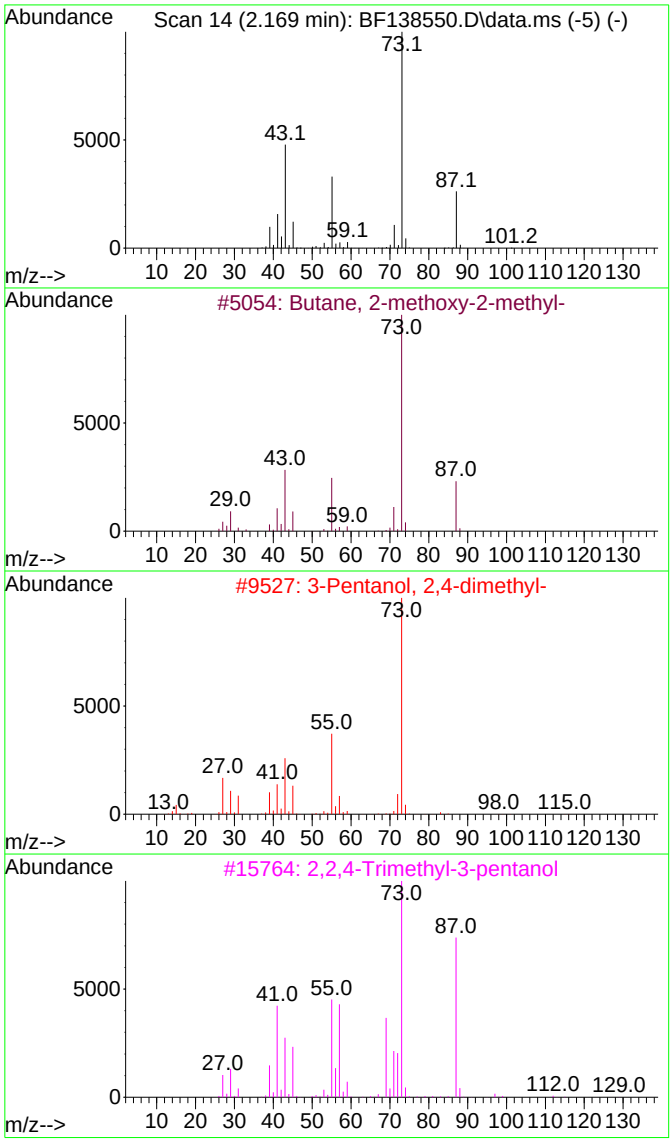
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

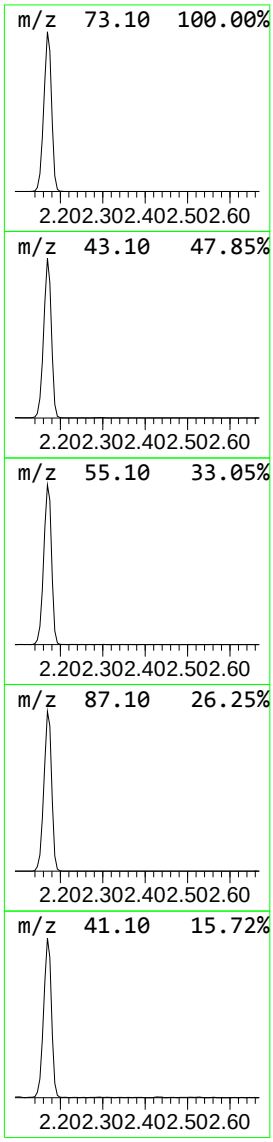
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	86.79 ng	2230840	1,4-Dichlorobenzene-d4	6.863

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

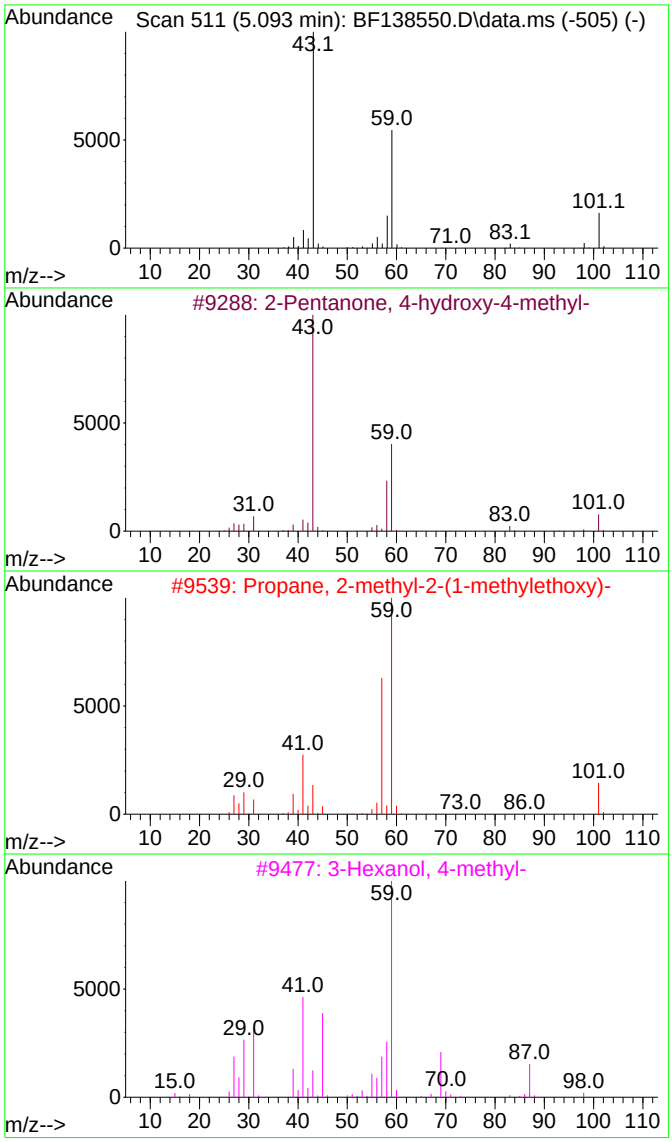
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

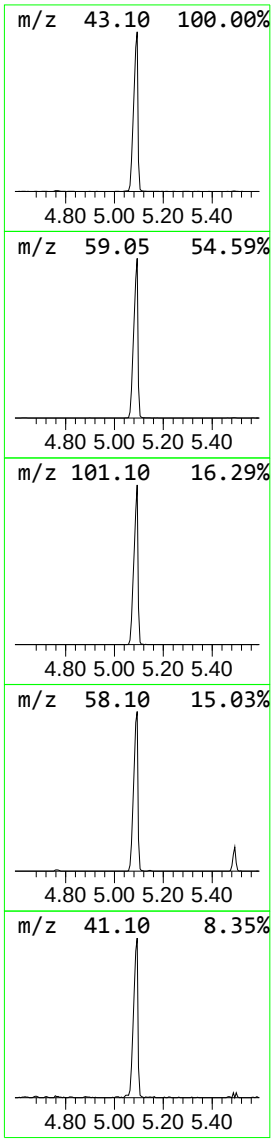
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	59.83 ng	1537750	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	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	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

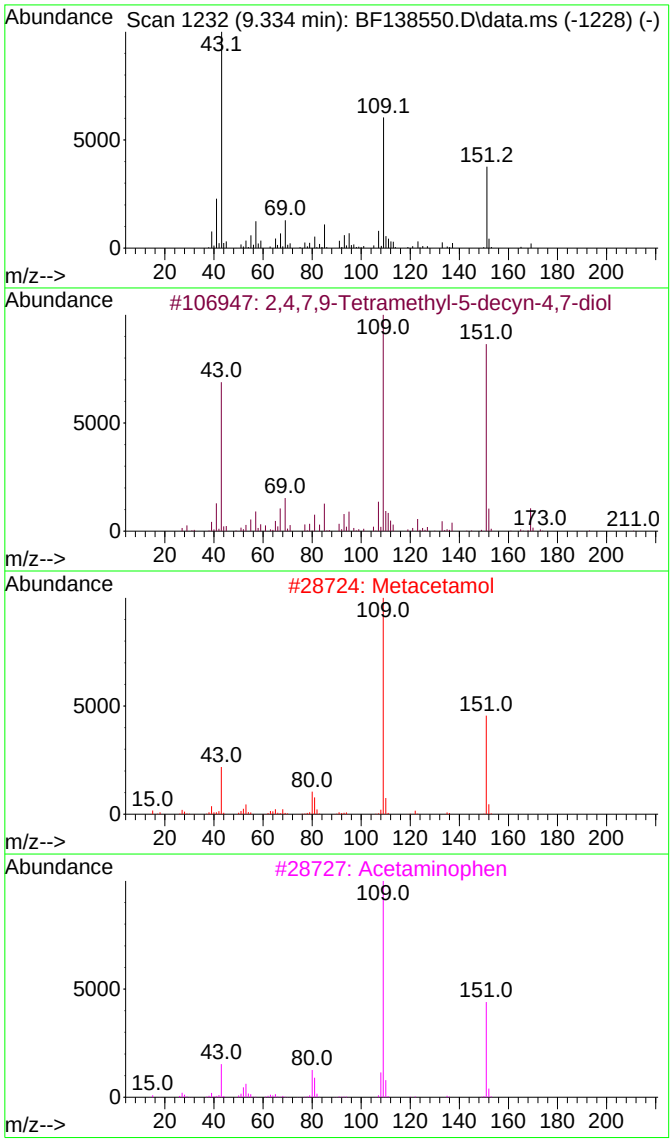
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

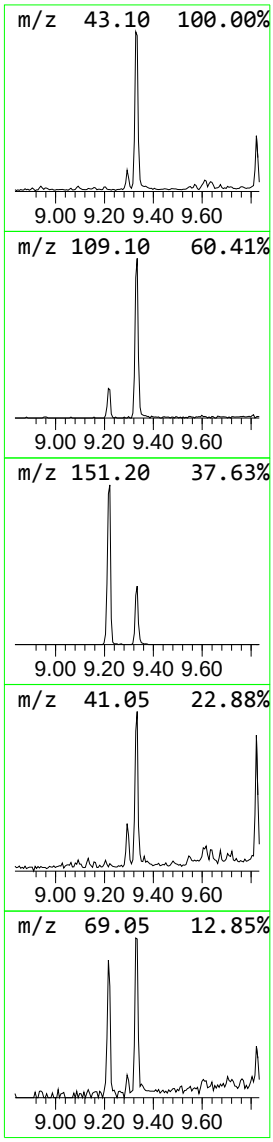
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.334	4.84 ng	173233	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Metacetamol	151	C8H9NO2	000621-42-1	47
3	Acetaminophen	151	C8H9NO2	000103-90-2	47
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
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Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

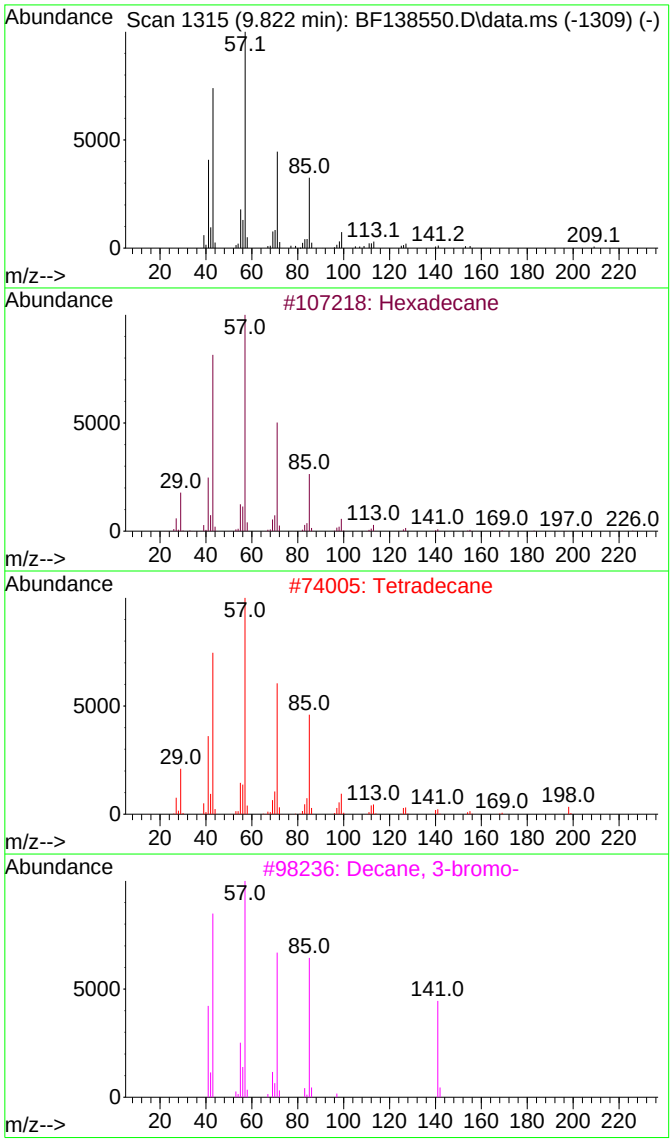
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

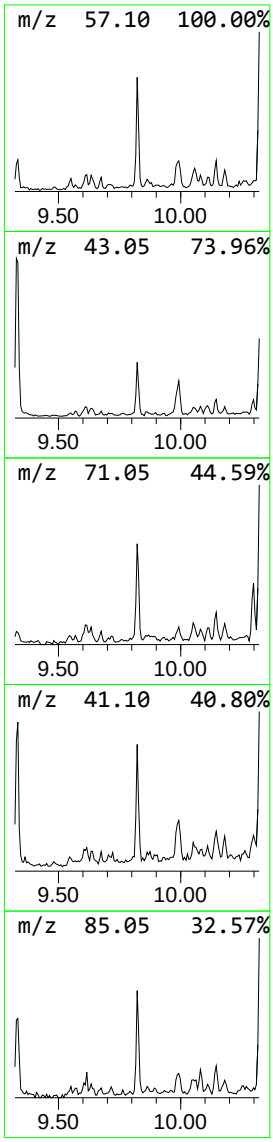
****

Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.822	2.10 ng	75116	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Decane, 3-bromo-	220	C10H21Br	030571-71-2	86
4	Tridecane	184	C13H28	000629-50-5	83
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

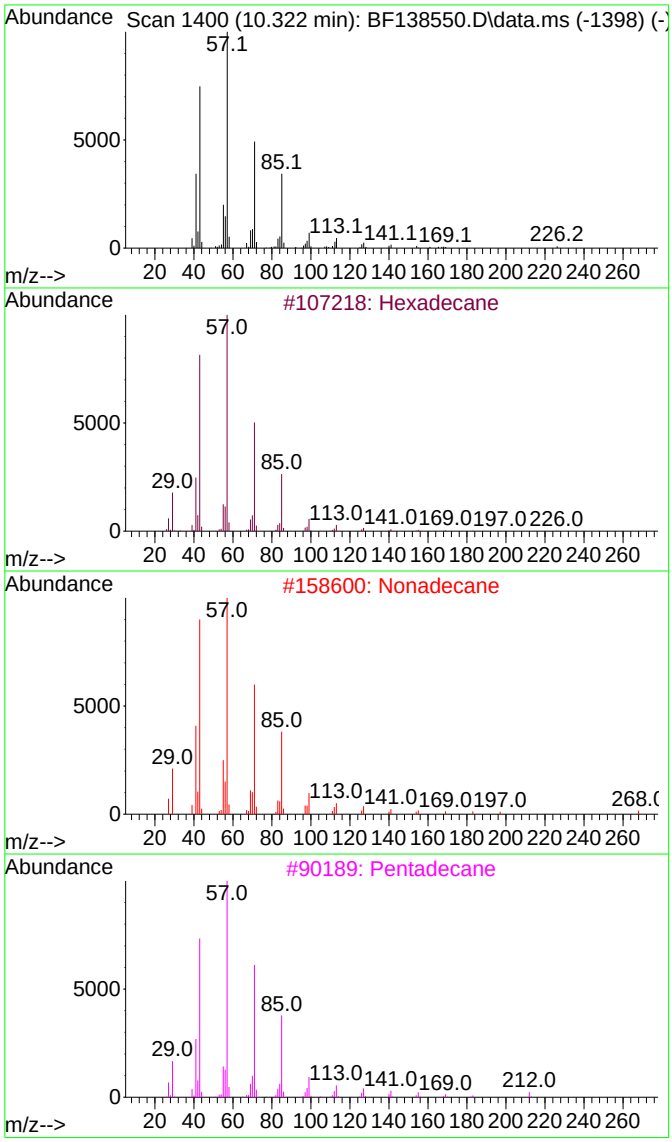
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

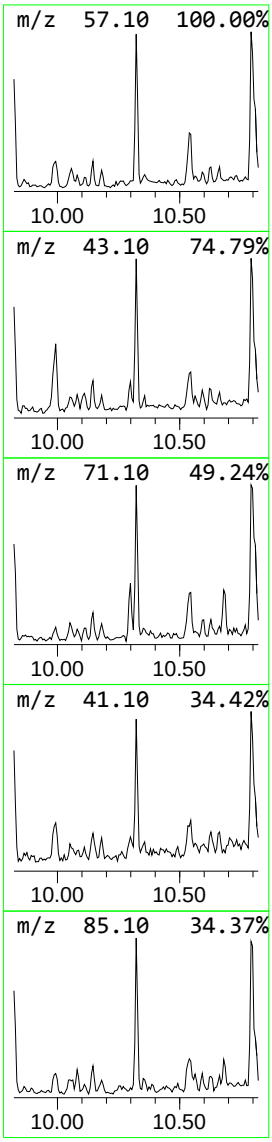
****

Peak Number 5 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.322	2.63 ng	94046	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Nonadecane	268	C19H40	000629-92-5	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	90
5	Tridecane	184	C13H28	000629-50-5	90





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Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
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Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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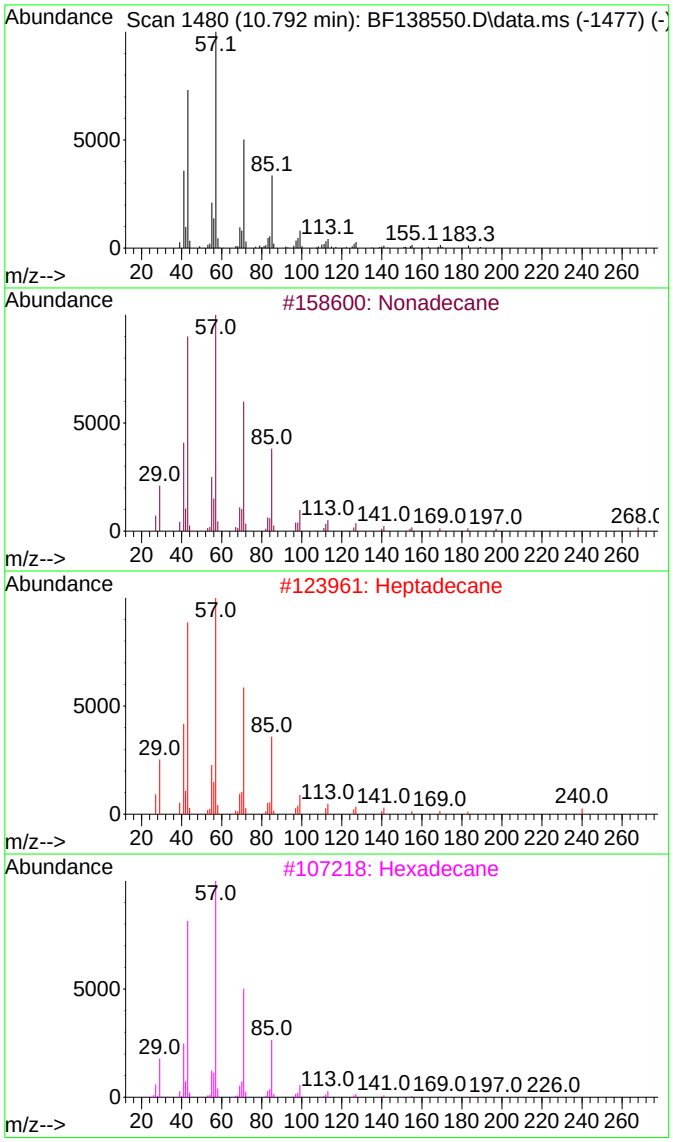
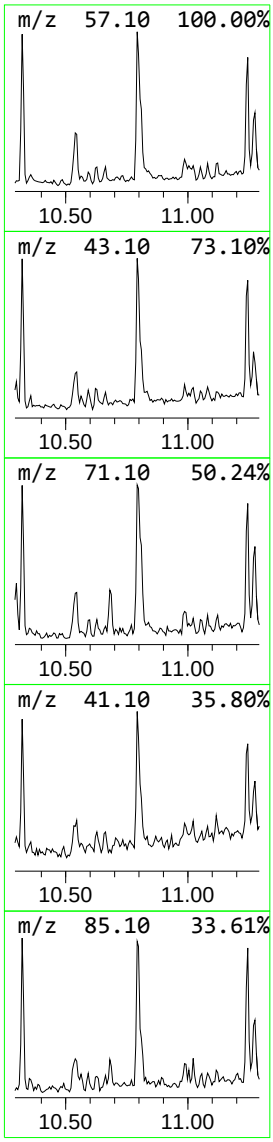
Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.792	5.05 ng	155034	Phenanthrene-d10	11.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86





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Misc :
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Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

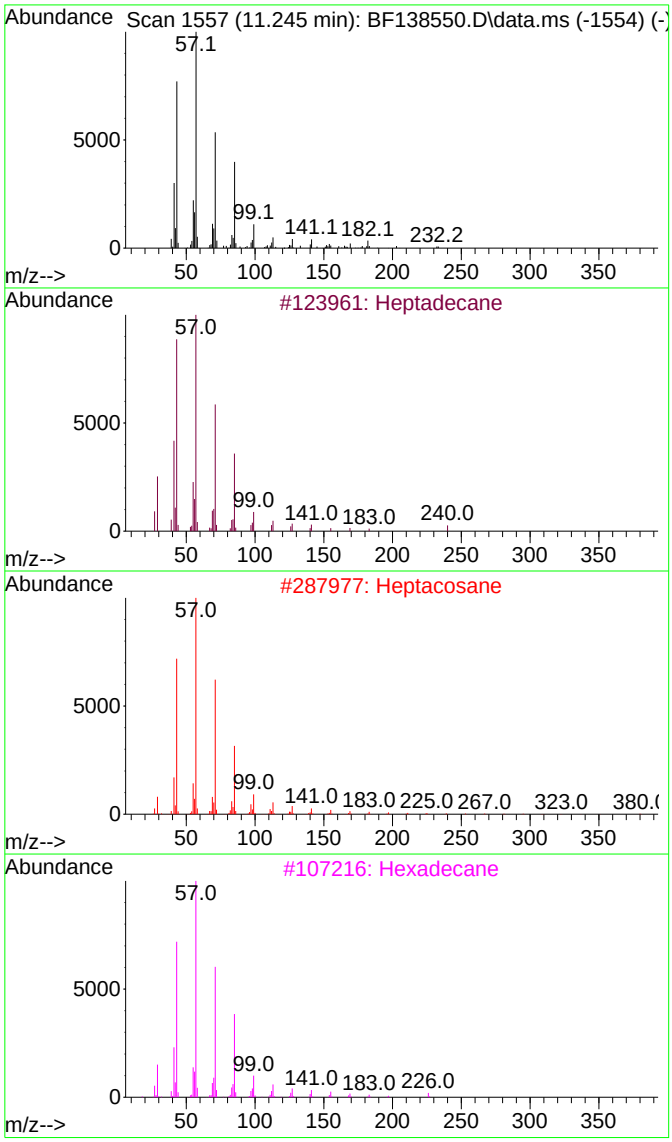
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

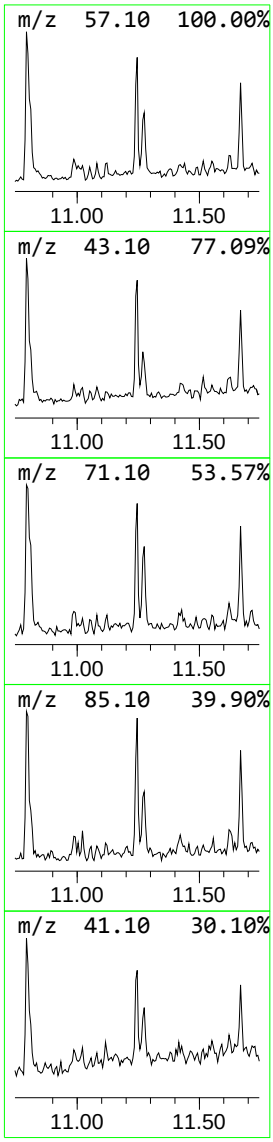
****

Peak Number 7 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.245	2.82 ng	86446	Phenanthrene-d10	11.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Tetracosane	338	C24H50	000646-31-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

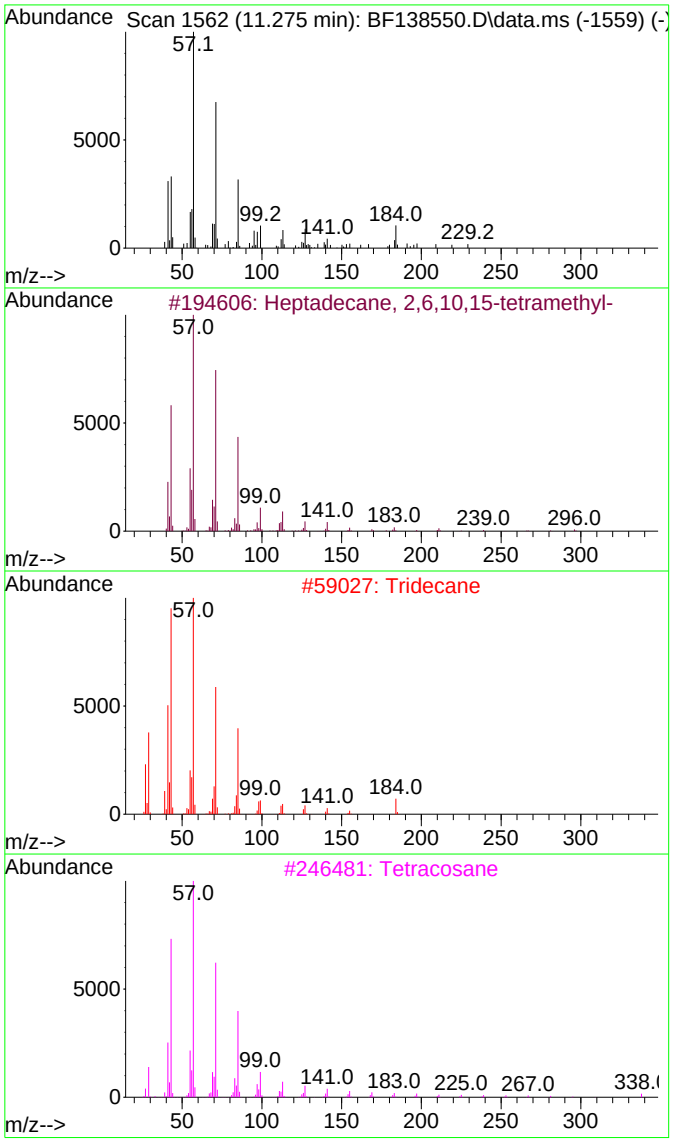
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

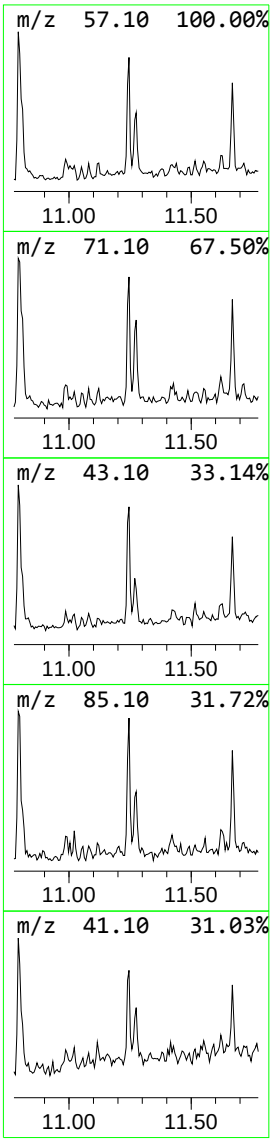
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptadecane, 2,6,10,15-tetr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.275	2.08 ng	63827	Phenanthrene-d10	11.381

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
2	Tridecane	184	C13H28	000629-50-5	80
3	Tetracosane	338	C24H50	000646-31-1	72
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
5	Octacosane	394	C28H58	000630-02-4	72





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Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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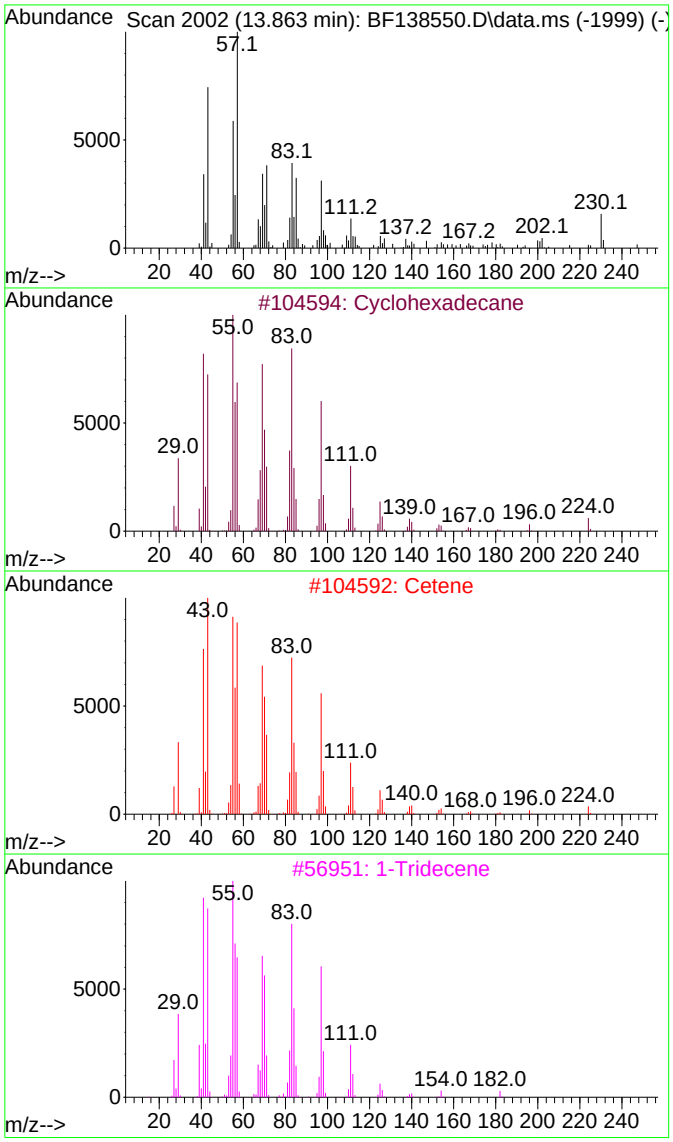
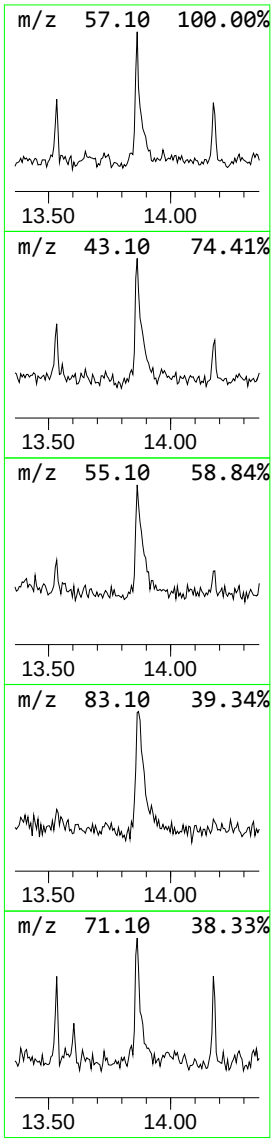
Peak Number 10 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	7.07 ng	165151	Chrysene-d12	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	93
2	Cetene	224	C16H32	000629-73-2	91
3	1-Tridecene	182	C13H26	002437-56-1	90
4	Propionic acid, 3-iodo-, heptade...	438	C20H39IO2	1000406-24-8	87
5	Propionic acid, 3-iodo-, octadec...	452	C21H41IO2	1000406-24-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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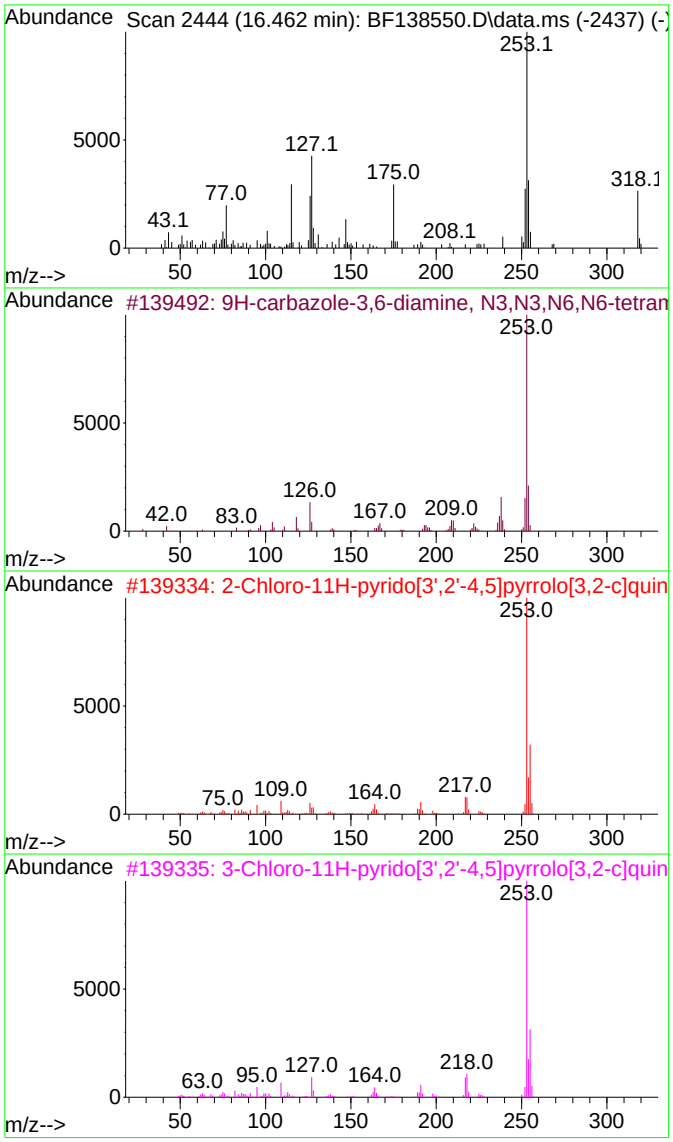
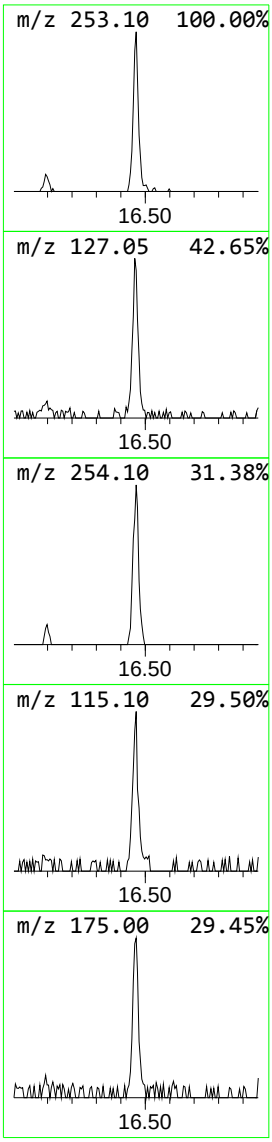
Peak Number 11 unknown16.462 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	5.59 ng	112371	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-carbazole-3,6-diamine, N3,N3,...	253	C16H19N3	1010396-68-8	46
2	2-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-3	27
3	3-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-4	27
4	Benzaldehyde, 4-((4-(dimethylami...	253	C15H15N3O	039208-00-9	22
5	4-Cyclopropyl-5-fluoro-1-oxobenz...	297	C17H12FNO3	1000435-59-2	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138550.D
Acq On : 12 Jul 2024 17:04
Operator : CG\JU
Sample : P3208-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONC-PADS

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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...	2.169	86.8	ng	2230840	1	6.863	514073	20.0
2-Pentanone, 4-...	5.093	59.8	ng	1537750	1	6.863	514073	20.0
2,4,7,9-Tetrame...	9.334	4.8	ng	173233	3	9.898	715573	20.0
Hexadecane	9.822	2.1	ng	75116	3	9.898	715573	20.0
Nonadecane	10.322	2.6	ng	94046	3	9.898	715573	20.0
Heptadecane	10.792	5.0	ng	155034	4	11.381	613572	20.0
Heptacosane	11.245	2.8	ng	86446	4	11.381	613572	20.0
Heptadecane, 2,...	11.275	2.1	ng	63827	4	11.381	613572	20.0
Cyclohexadecane	13.863	7.1	ng	165151	5	14.016	467477	20.0
unknown16.462	16.462	5.6	ng	112371	6	15.480	401856	20.0