LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

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-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130200.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	20	26	33	rVB3	48347	104485	1.83%	0.252%
2	3.222	145	159	165	rBV2	55499	139395	2.45%	0.336%
3	3.387	177	187	193	rBV2	52987	115285	2.02%	0.278%
4	3.710	234	242	246	rBV	39094	60594	1.06%	0.146%
5	4.152	309	317	327	rVB2	174236	255091	4.48%	0.614%
6	4.240	327	332	336	rBV	158897	189503	3.33%	0.456%
7	4.393	350	358	367	rBV	187365	238146	4.18%	0.573%
8	4.657	398	403	405	rBV2	53575	70348	1.23%	0.169%
9	4.875	436	440	448	rBV2	117038	147659	2.59%	0.355%
10	5.293	507	511	514	rVB	2041916	1873174	32.87%	4.509%
11	5.857	602	607	610	rBV	428449	376266	6.60%	0.906%
12	6.151	654	657	660	rVB	389269	314157	5.51%	0.756%
13	6.322	681	686	691	rVB	1354949	1235968	21.69%	2.975%
14	6.375	691	695	697	rBV	86655	70640	1.24%	0.170%
15	6.634	734	739	745	rVB2	136861	170864	3.00%	0.411%
16	6.693	745	749	752	rBV	1027444	797101	13.99%	1.919%
17	6.816	767	770	773	rBV	115714	84019	1.47%	0.202%
18	6.875	776	780	783	rVB	1659566	1427305	25.04%	3.436%
19	6.946	789	792	794	rBV	134704	109285	1.92%	0.263%
20	7.016	800	804	805	rBV	71692	66608	1.17%	0.160%
21	7.034	805	807	811	rVB	218323	174589	3.06%	0.420%
22	7.087	812	816	821	rBV	69726	69074	1.21%	0.166%
23	7.169	826	830	833	rVB	269133	231119	4.06%	0.556%
24	7.263	834	846	849	rBV	3296575	3729700	65.44%	8.978%
25	7.381	854	866	868	rBV4	568575	1291228	22.66%	3.108%
26	7.463	871	880	882	rBV	840764	1760505	30.89%	4.238%
27	7.663	912	914	918	rVB	155431	134545	2.36%	0.324%
28	7.710	918	922	928	rVB3	87363	107823	1.89%	0.260%
29	7.840	933	944	946	rBV	807723	1484584	26.05%	3.574%
30	7.910	952	956	961	rVB3	106416	160978	2.82%	0.387%
31	7.975	961	967	969	rBV	1564393	1365419	23.96%	3.287%
32	7.998	969	971	974	rVB2	188348	153150	2.69%	0.369%
33	8.145	991	996	999	rBV2	202417	260130	4.56%	0.626%
34	8.204	999	1006	1011	rVB5	312026	453176	7.95%	1.091%
35	8.269	1011	1017	1021	rBV3	191425	274077	4.81%	0.660%
36	8.375	1029	1035	1037	rBV2	300113	454044	7.97%	1.093%

LSC Area Percent Report

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Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP090822

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-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.428	1037	1044	1046	rBV2	406433	549429	9.64%	1.323%
38	8.534	1058	1062	1065	rBV	172786	133677	2.35%	0.322%
39	8.640	1078	1080	1083	rVB	88642	61589	1.08%	0.148%
40	8.740	1093	1097	1100	rBV3	78288	121110	2.13%	0.292%
41	8.781	1100	1104	1107	rVB2	68207	96678	1.70%	0.233%
42	9.051	1145	1150	1153	rBV	6200969	5699075	100.00%	13.718%
43	9.528	1228	1231	1236	rVB3	113890	131055	2.30%	0.315%
44	9.581	1237	1240	1244	rBV	97411	81349	1.43%	0.196%
45	9.639	1244	1250	1253	rBV	519981	664694	11.66%	1.600%
46	9.722	1259	1264	1267	rBV	1791339	1464647	25.70%	3.526%
47	9.757	1267	1270	1277	rVB	116083	117175	2.06%	0.282%
48	9.869	1285	1289	1295	rBV	207870	215371	3.78%	0.518%
49	9.922	1295	1298	1302	rVB4	52208	78570	1.38%	0.189%
50	10.039	1316	1318	1323	rVB	64921	63377	1.11%	0.153%
51	10.086	1323	1326	1329	rBV	181559	162127	2.84%	0.390%
52	10.510	1393	1398	1401	rBV	3985913	3645244	63.96%	8.775%
53	11.204	1512	1516	1519	rBV	1562054	1283388	22.52%	3.089%
54	11.739	1603	1607	1611	rBV	233068	217344	3.81%	0.523%
55	12.410	1718	1721	1723	rBV	90521	76059	1.33%	0.183%
56	12.522	1737	1740	1752	rVB	112151	127555	2.24%	0.307%
57	12.792	1781	1786	1789	rBV	4888737	4374303	76.75%	10.529%
58	13.745	1944	1948	1958	rVB3	51971	96562	1.69%	0.232%
59	13.833	1959	1963	1966	rBV	911485	874020	15.34%	2.104%
60	15.227	2196	2200	2205	rBV	782662	931149	16.34%	2.241%
61	15.274	2205	2208	2213	rVB	50120	66057	1.16%	0.159%
62	15.674	2273	2276	2284	rVB	48887	69416	1.22%	0.167%
63	16.139	2352	2355	2364	rVB3	50019	84060	1.47%	0.202%
64	17.321	2551	2556	2564	rVB6	40073	108320	1.90%	0.261%

Sum of corrected areas: 41543434

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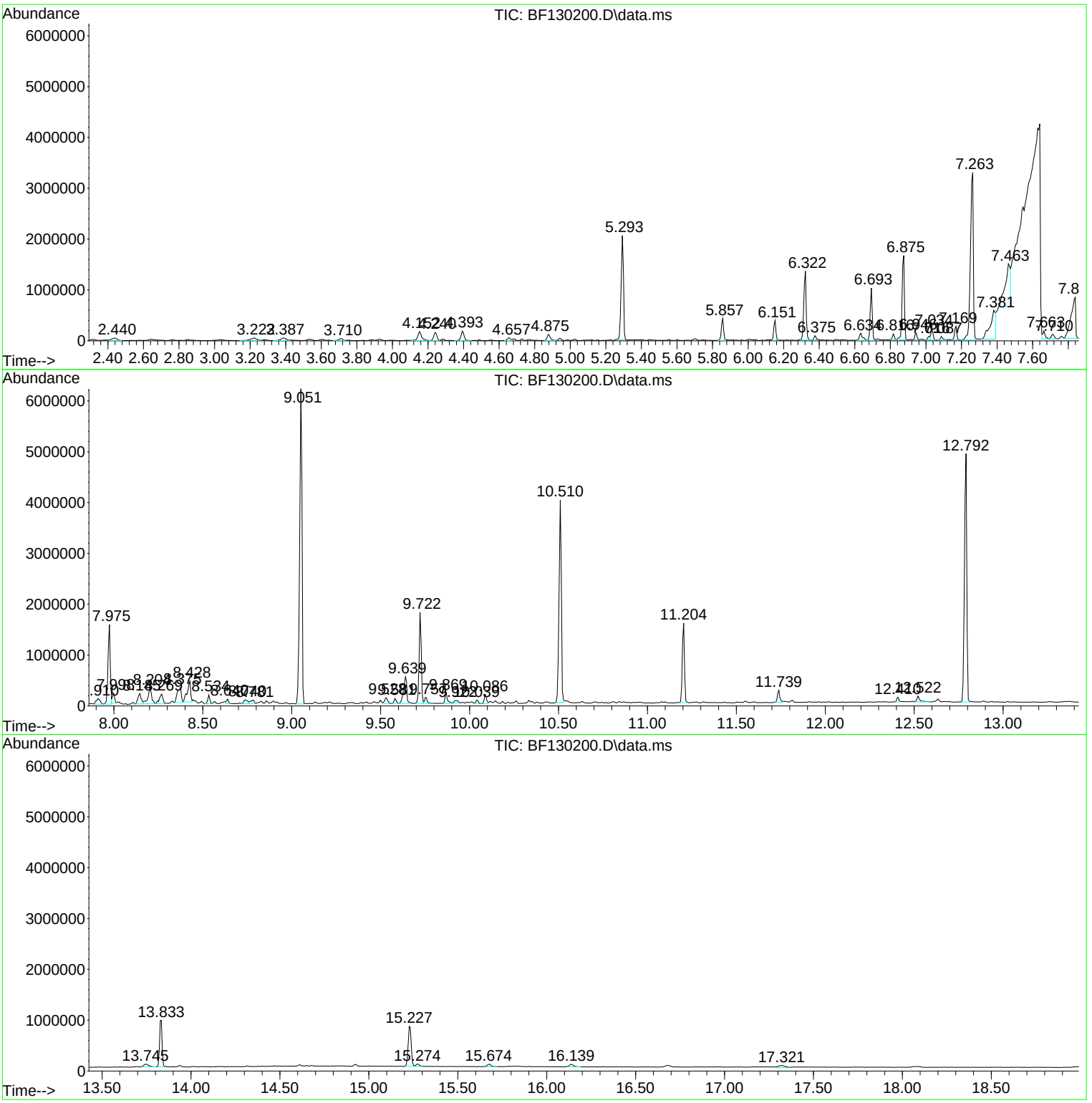
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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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Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
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Instrument :
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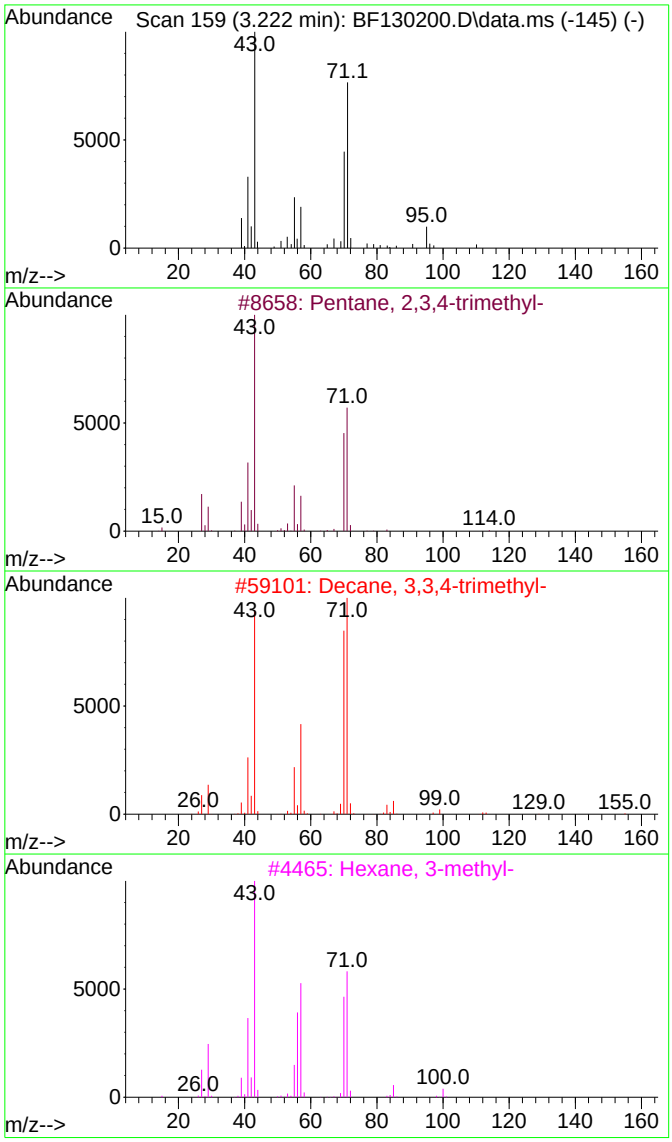
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

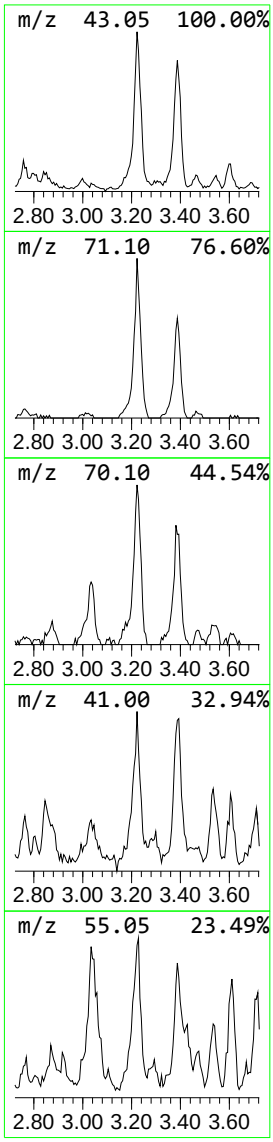
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3,4-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.222	3.50 ng	139395	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	86
2	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	72
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	72
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

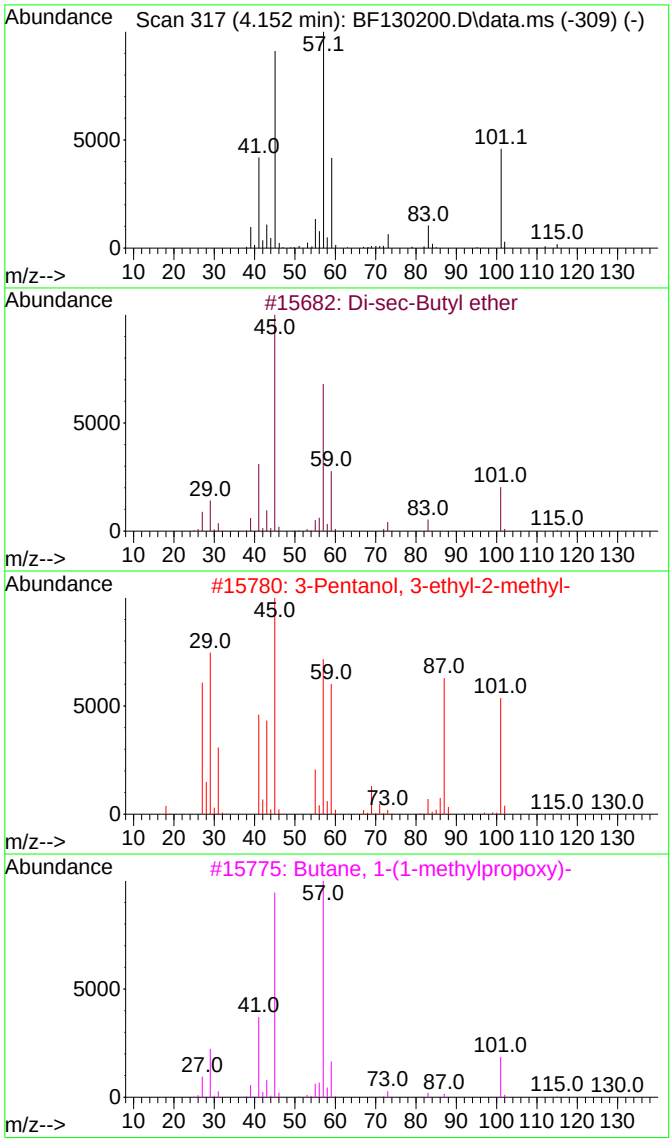
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

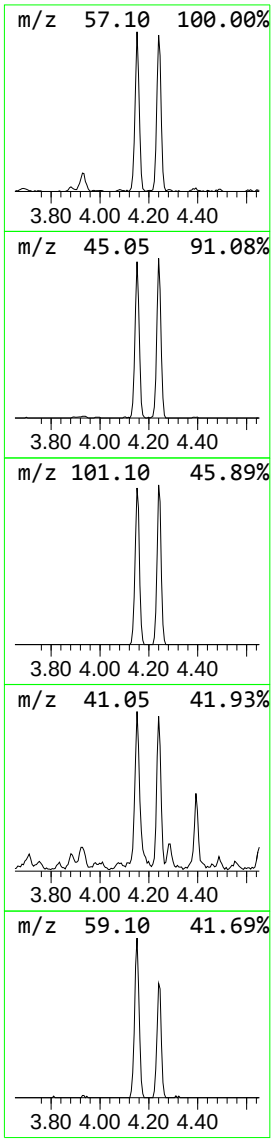
****

Peak Number 2 Di-sec-Butyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.152	6.40 ng	255091	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	56
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
4	Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	38
5	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
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Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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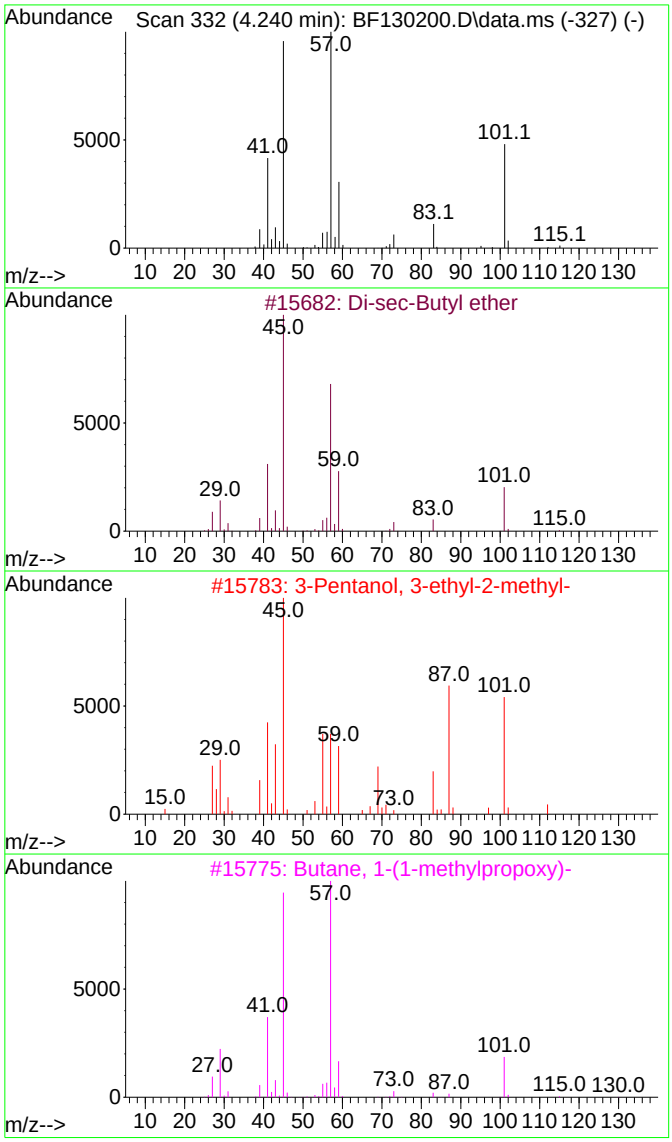
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

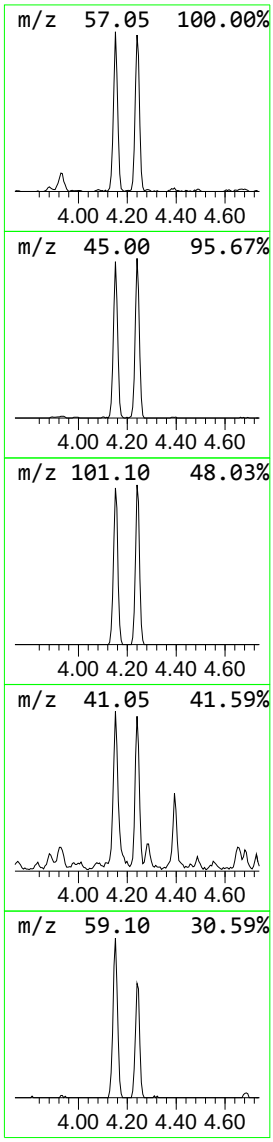
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Pentanol, 3-ethyl-2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	4.75 ng	189503	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	72
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	45
5	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

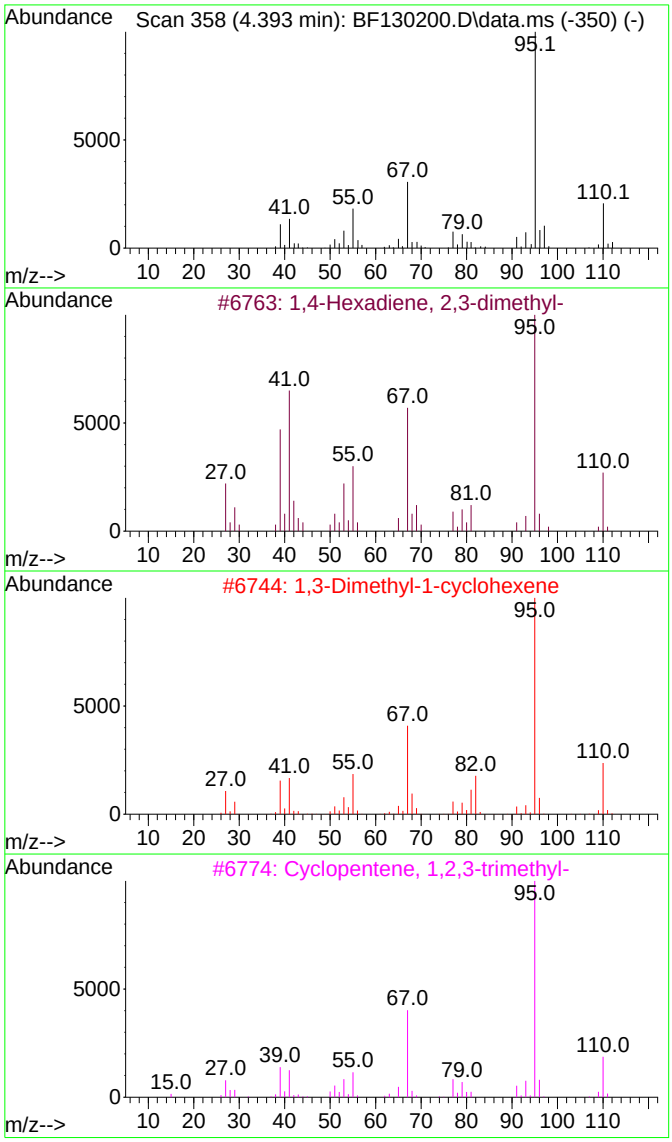
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

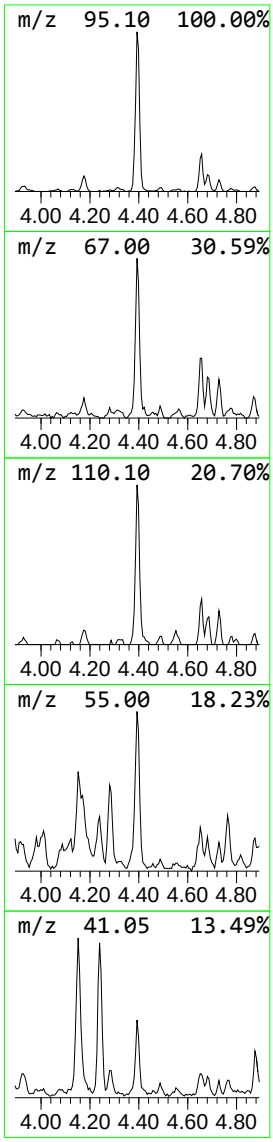
****

Peak Number 4 1,4-Hexadiene, 2,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.393	5.98 ng	238146	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	87
2	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	83
3	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	83
4	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	64
5	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
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Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

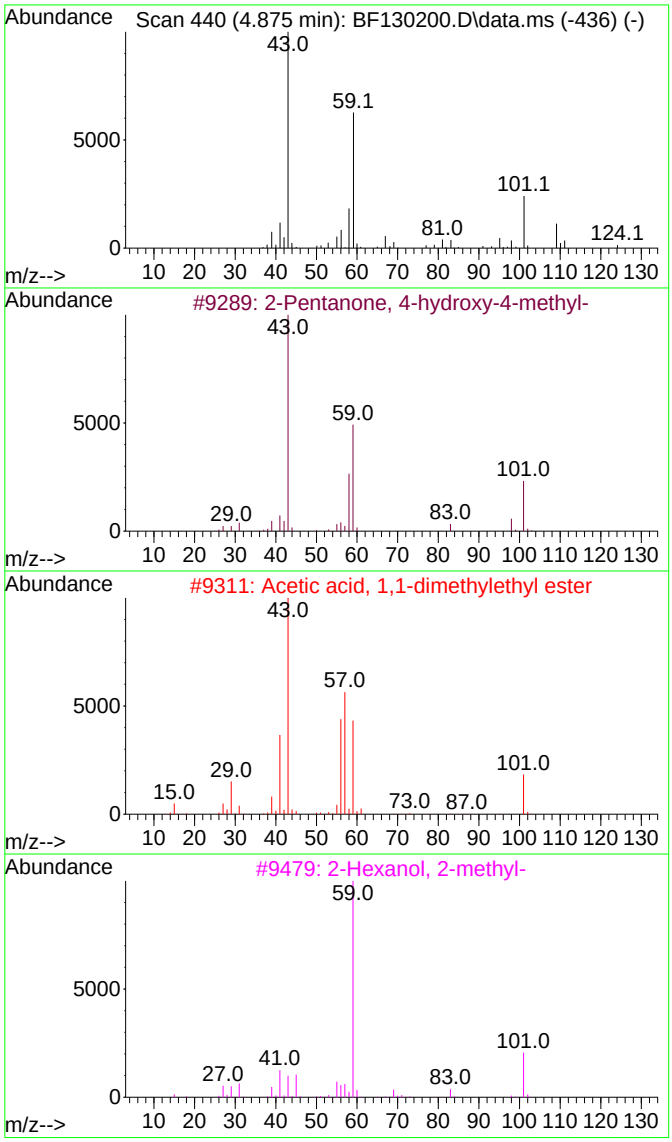
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

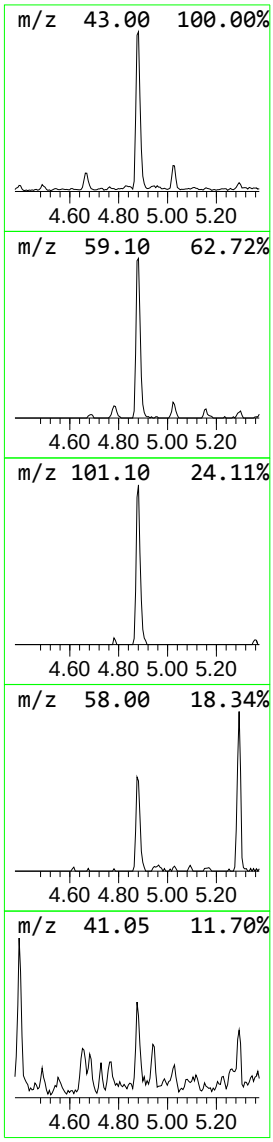
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	3.70 ng	147659	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	32
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	25
5	1-Cyclohexylethanol, methyl ether	142	C9H18O	1000365-12-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
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Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

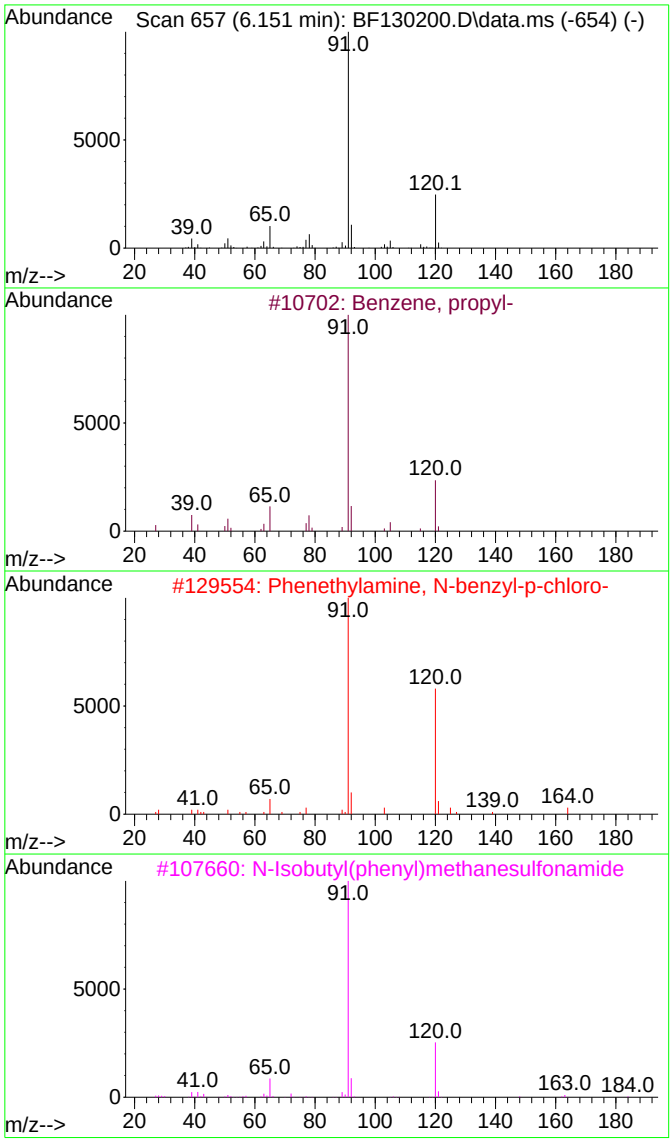
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

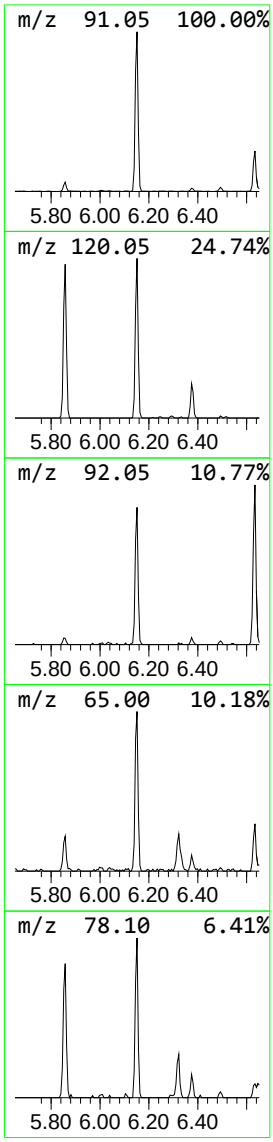
****

Peak Number 7 Benzene, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.151	7.88 ng	314157	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	94
2	Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	72
3	N-Isobutyl(phenyl)methanesulfona...	227	C11H17NO2S	144615-94-1	72
4	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	72
5	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

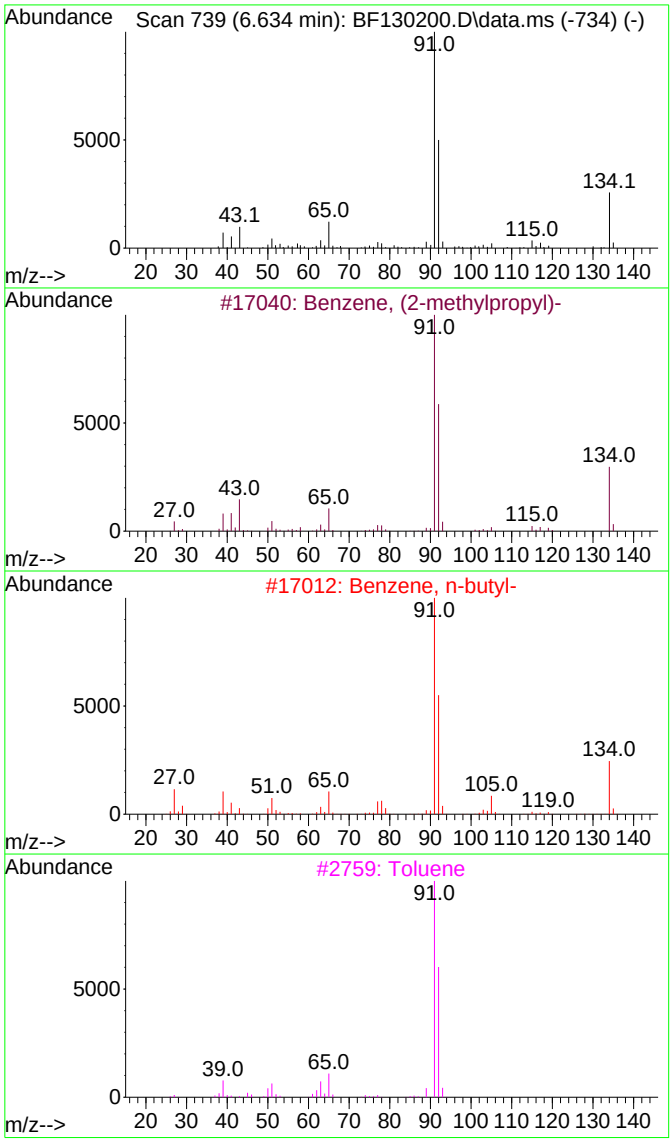
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

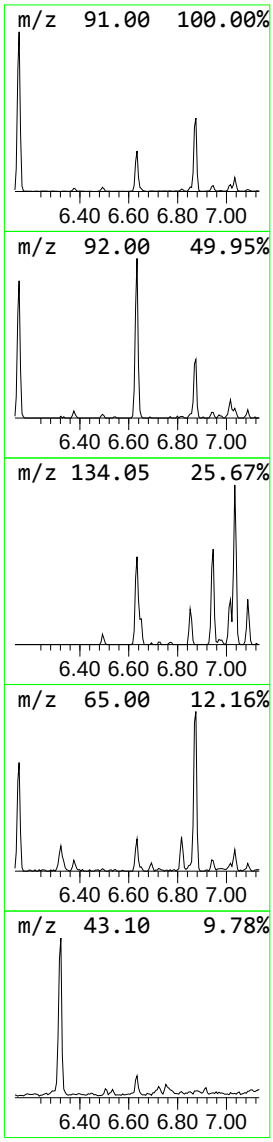
****

Peak Number 8 Benzene, (2-methylpropyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.634	4.29 ng	170864	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methylpropyl)-	134	C10H14	000538-93-2	90
2	Benzene, n-butyl-	134	C10H14	000104-51-8	80
3	Toluene	92	C7H8	000108-88-3	52
4	(3-Bromo-1-methylpropoxymethyl)b...	242	C11H15BrO	051666-29-6	50
5	Tetracyclo[3.2.0.0(2,7).0(4,6)]h...	92	C7H8	000278-06-8	46





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Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

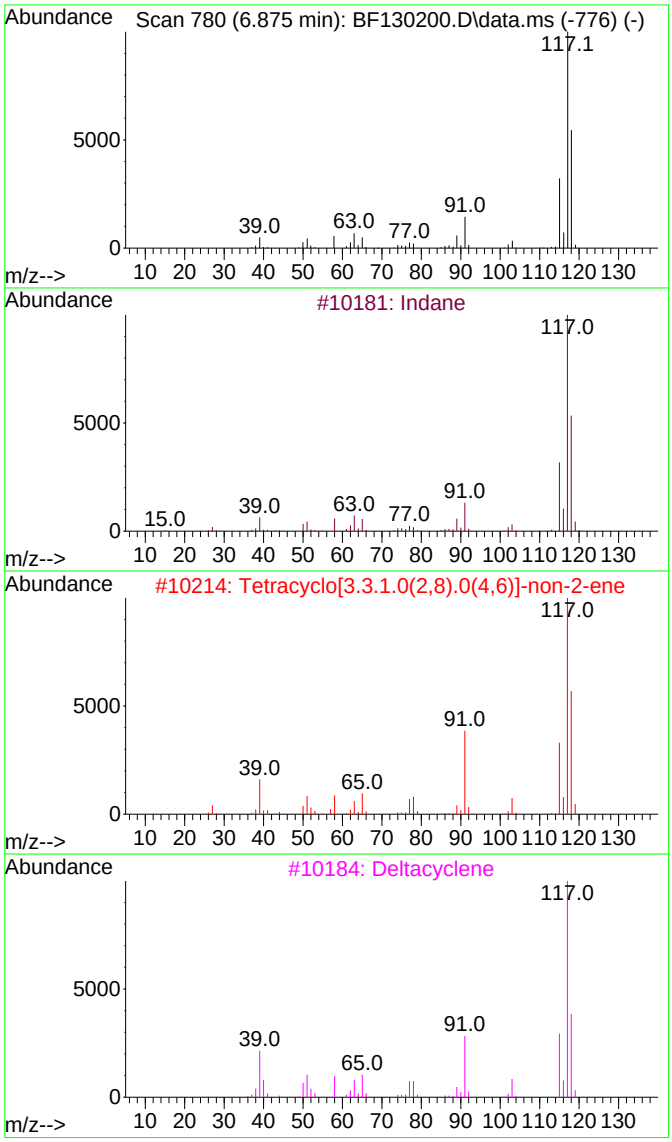
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

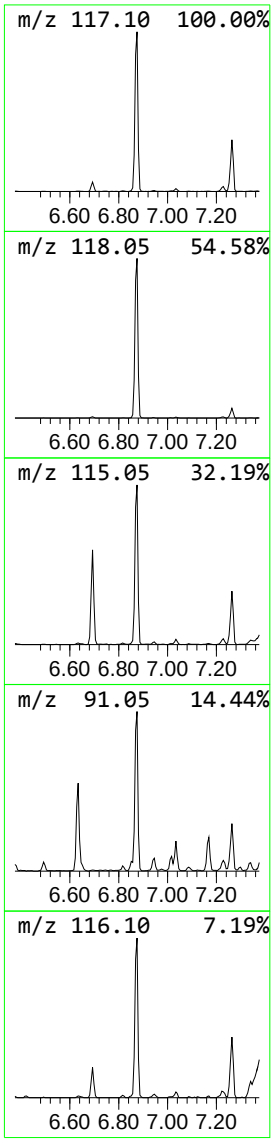
****

Peak Number 9 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.875	35.81 ng	1427310	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
3	Deltacyclene	118	C9H10	007785-10-6	64
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	59





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Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

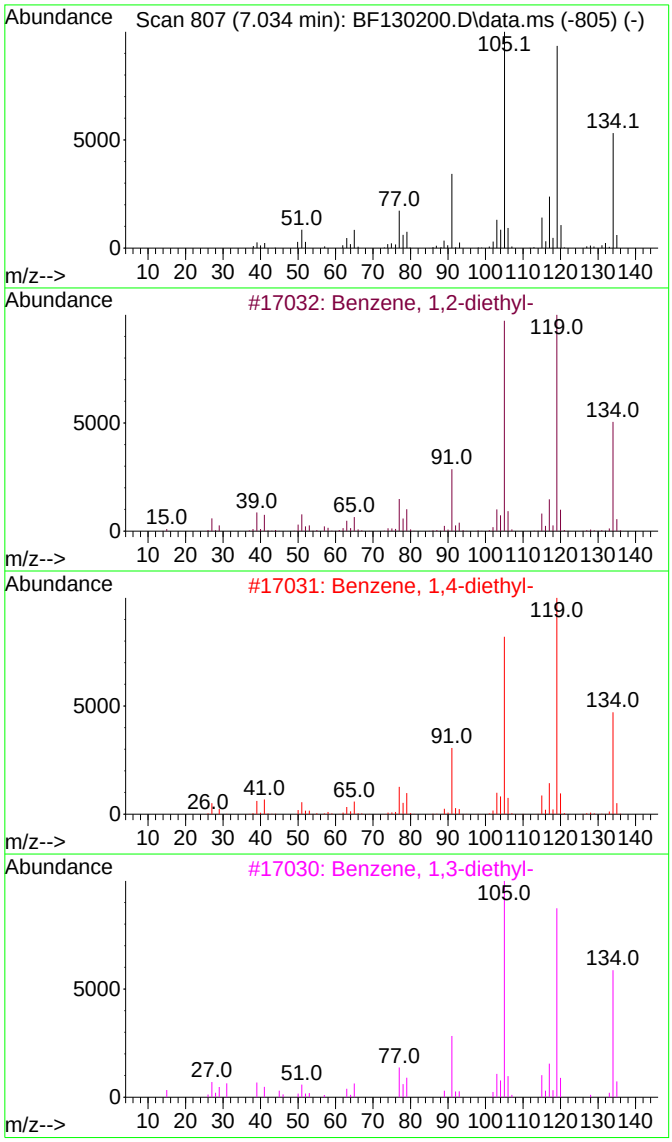
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

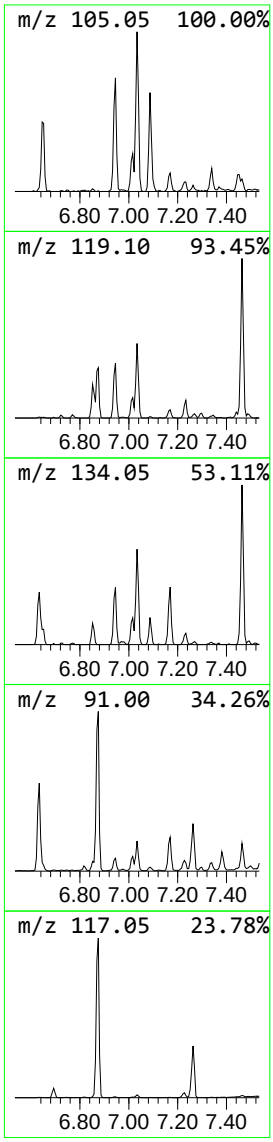
****

Peak Number 10 Benzene, 1,2-diethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	4.38 ng	174589	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	94
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	91
3	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	91
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	83





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Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

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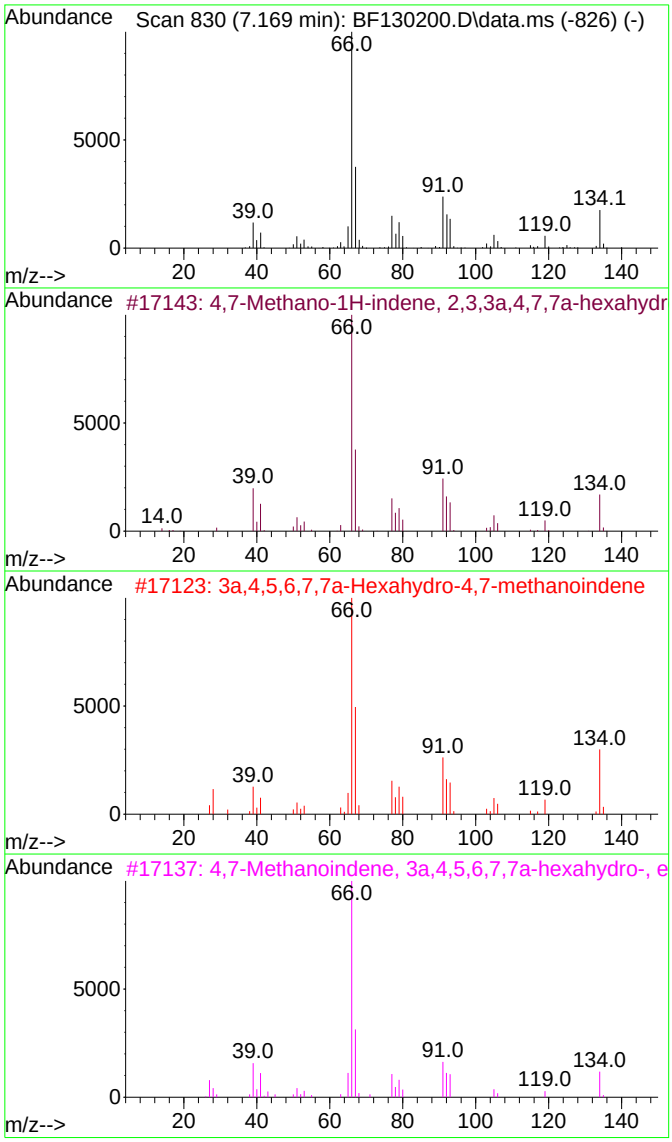
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

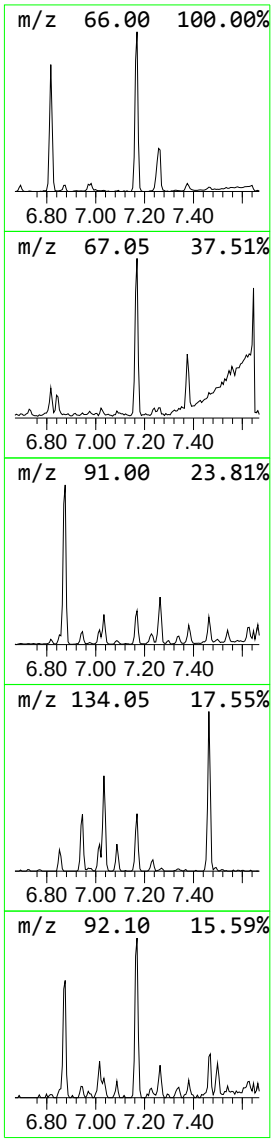
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 4,7-Methano-1H-indene, 2,3,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.169	5.80 ng	231119	1,4-Dichlorobenzene-d4	6.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-1H-indene, 2,3,3a,4,...	134	C10H14	002826-19-9	96
2	3a,4,5,6,7,7a-Hexahydro-4,7-meth...	134	C10H14	004488-57-7	95
3	4,7-Methanoindene, 3a,4,5,6,7,7a...	134	C10H14	002825-86-7	95
4	5-Allyl-2-norbornene	134	C10H14	031663-53-3	91
5	Spiro[bicyclo[2.2.1]hept-5-ene-2...	120	C9H12	006572-50-5	72





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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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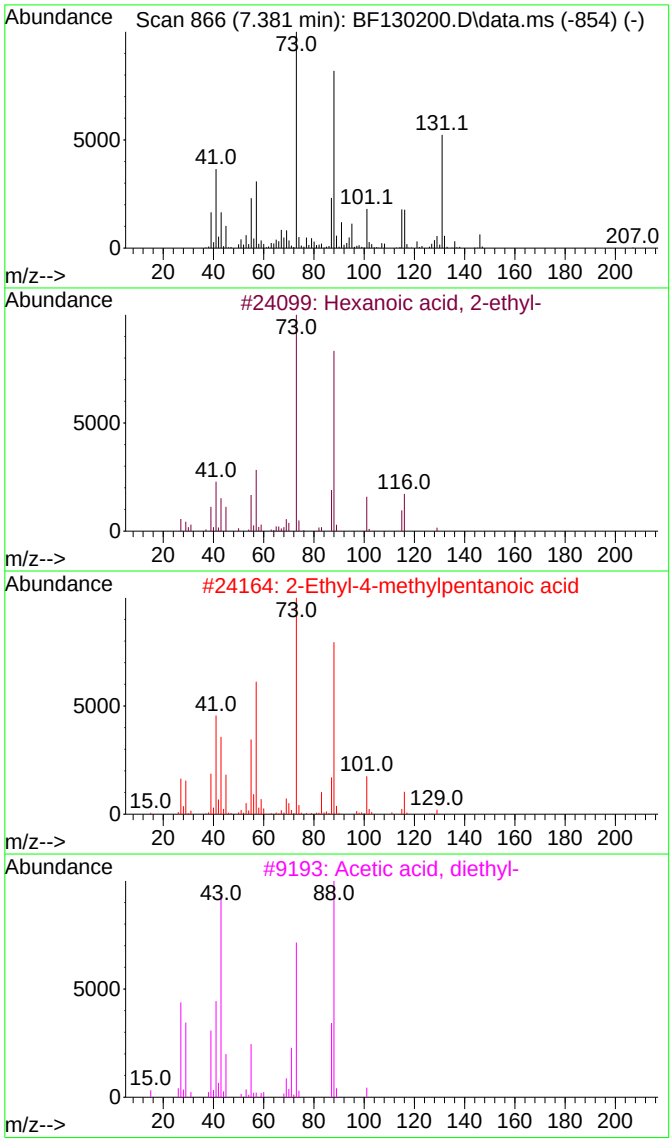
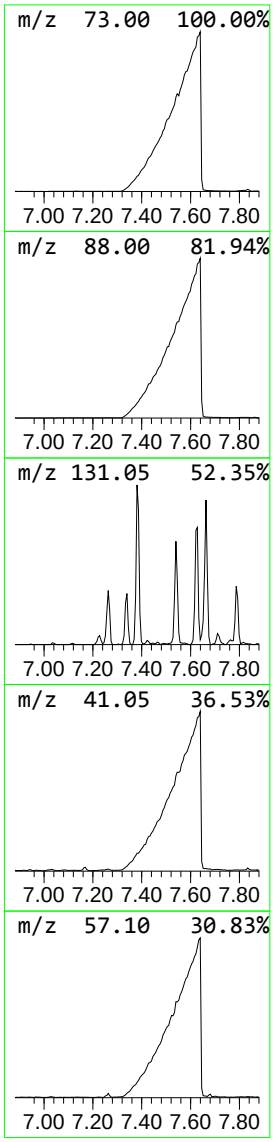
Peak Number 12 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.381	18.91 ng	1291230	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	58
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	53
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	43
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	37
5	Butyl mannoside, tetramethyl ether	292	C14H28O6	1000501-84-1	35





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Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

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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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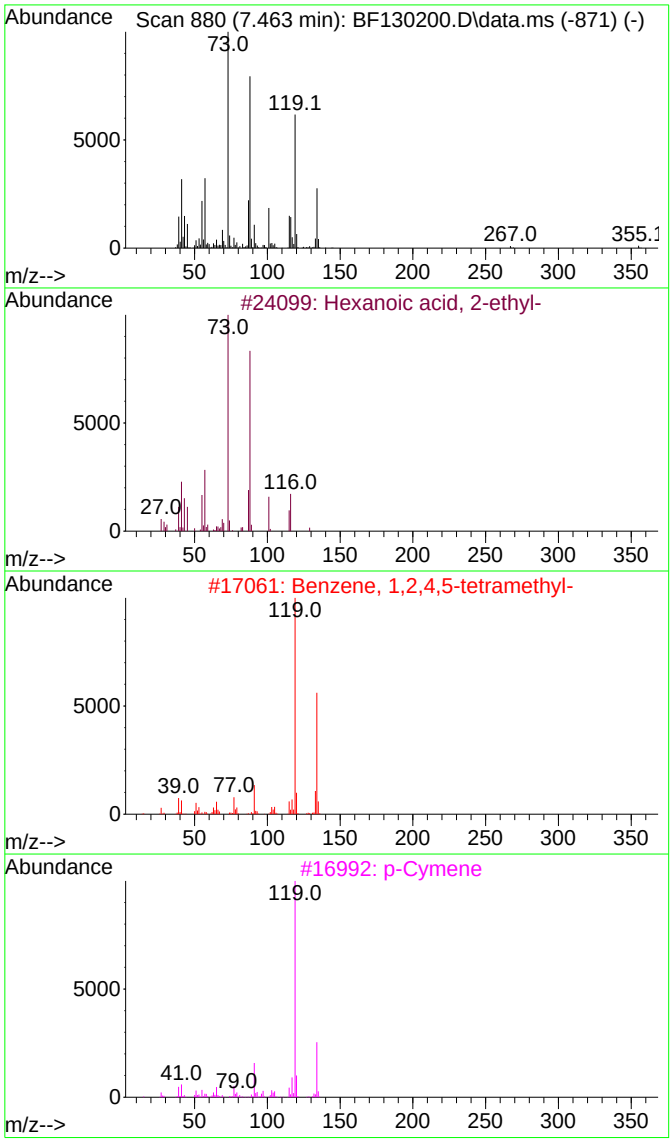
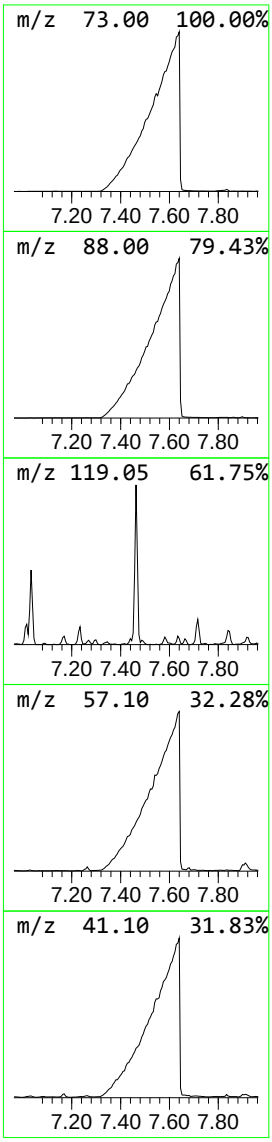
Peak Number 13 unknown7.463 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.463	25.79 ng	1760510	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	52
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	38
3	p-Cymene	134	C10H14	000099-87-6	35
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	35
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	35





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Sample : N4549-21
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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

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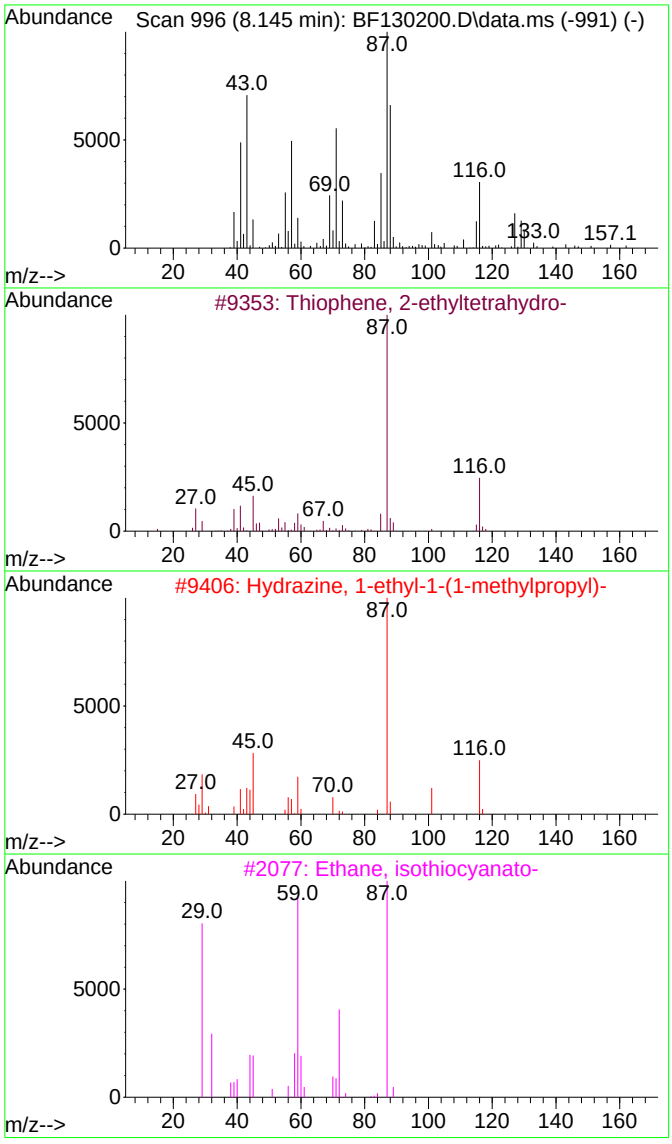
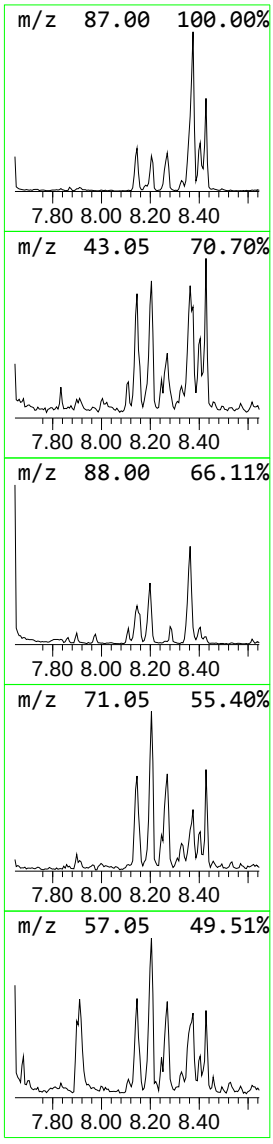
Peak Number 14 unknown8.145 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.145	3.81 ng	260130	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	35
2	Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	35
3	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	25
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	22
5	Acetic acid, 3-ethylpent-3-yl ester	158	C9H18O2	1000368-76-0	22





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Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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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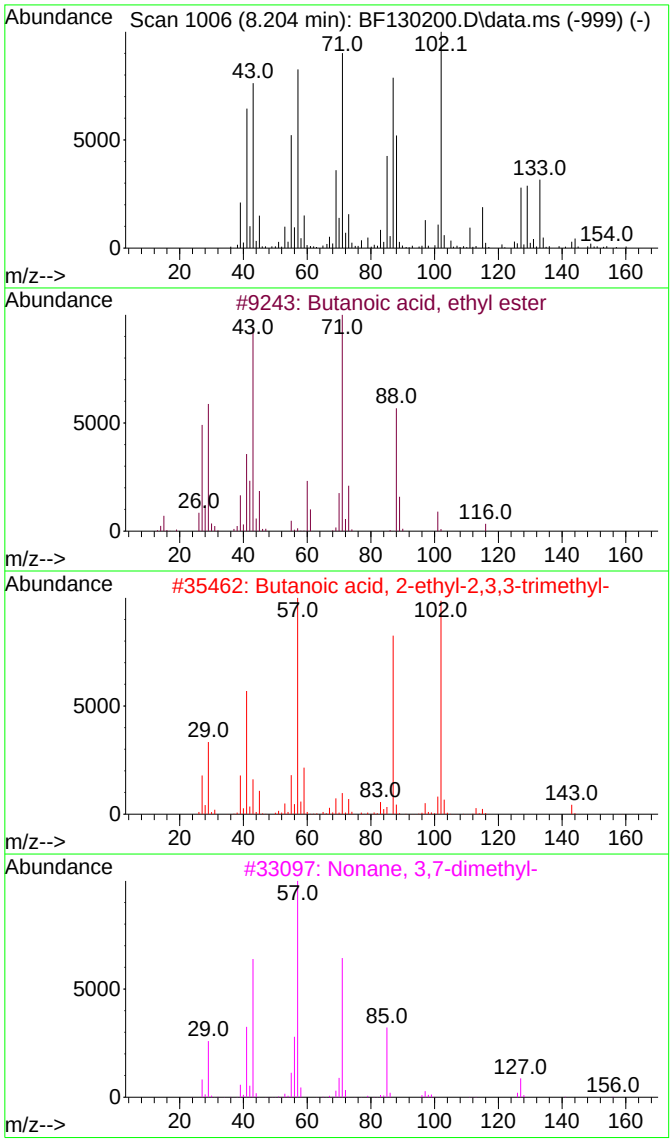
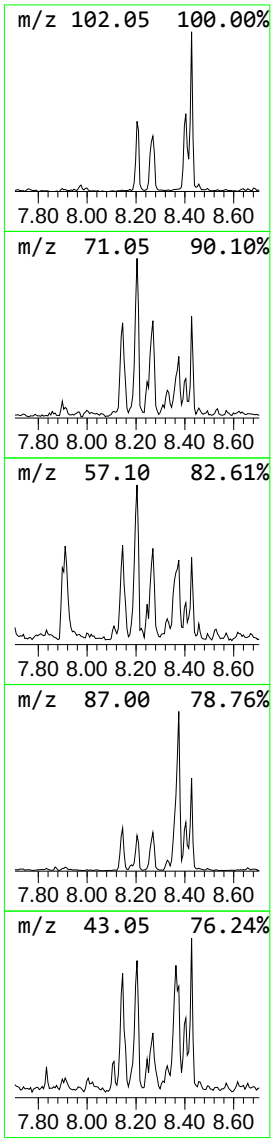
Peak Number 15 unknown8.204 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.204	6.64 ng	453176	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	35
2	Butanoic acid, 2-ethyl-2,3,3-tri...	158	C9H18O2	038541-67-2	35
3	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	22
4	Pentanoic acid, 2-ethyl-, methyl...	144	C8H16O2	000816-16-0	22
5	Pentanoic acid, 2-methyl-, ethyl...	144	C8H16O2	039255-32-8	22





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Operator : CG\JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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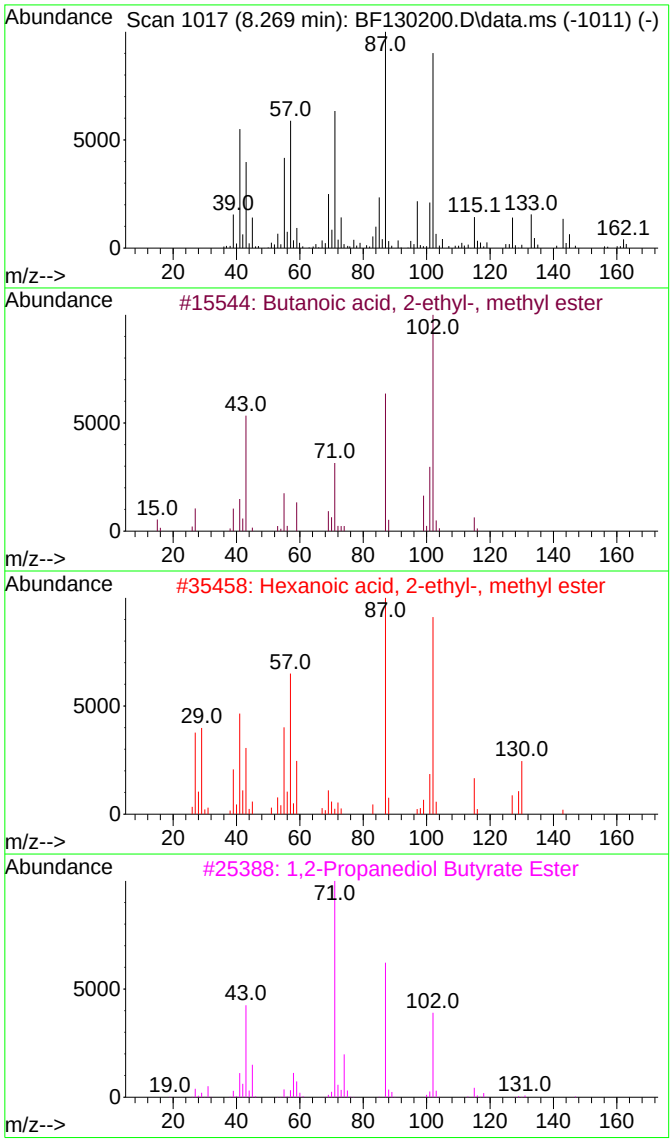
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

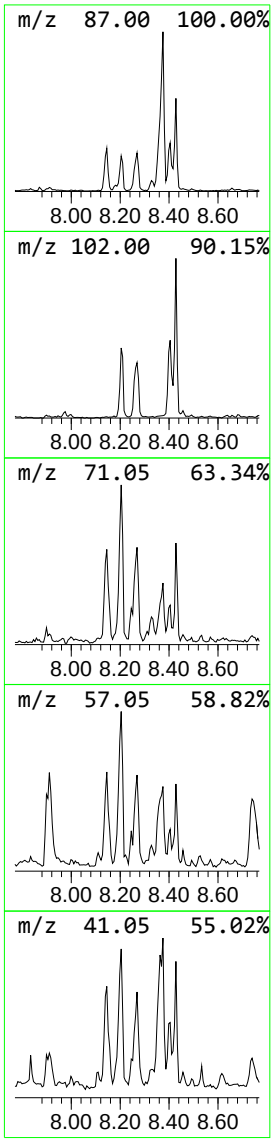
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Butanoic acid, 2-ethyl-, me... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.269	4.01 ng	274077	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	50
2	Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	47
3	1,2-Propanediol Butyrate Ester	146	C7H14O3	1000458-47-4	43
4	Pentanoic acid, 2-ethyl-, methyl...	144	C8H16O2	000816-16-0	38
5	Decanoic acid, 3-methyl-	186	C11H22O2	060308-82-9	32





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ALS Vial : 10 Sample Multiplier: 1

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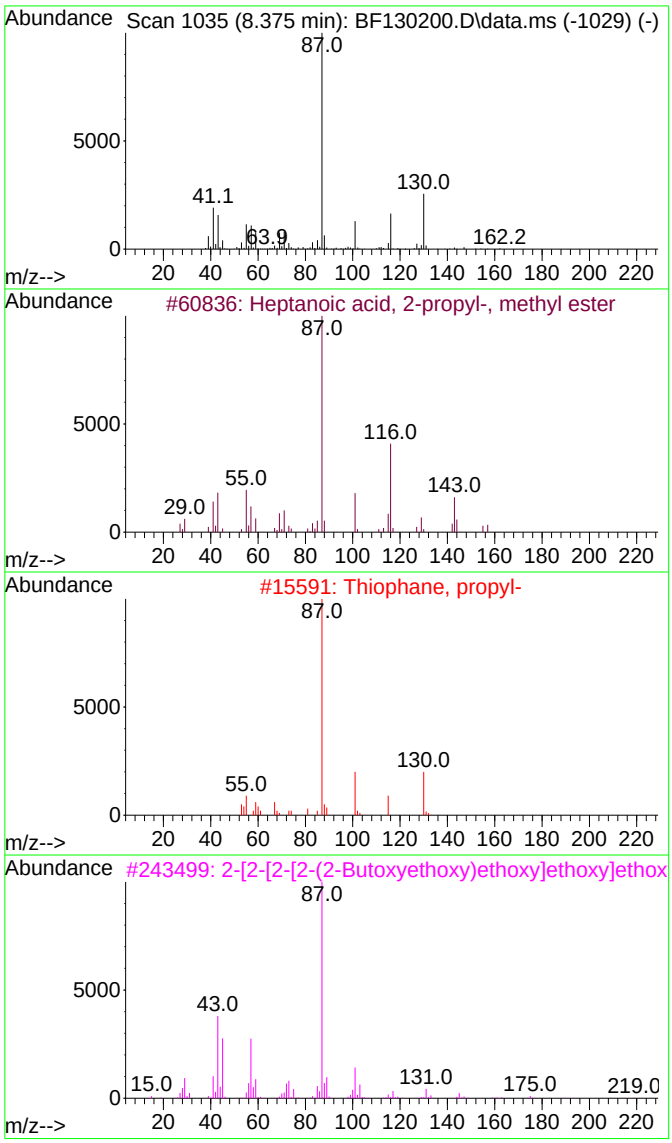
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

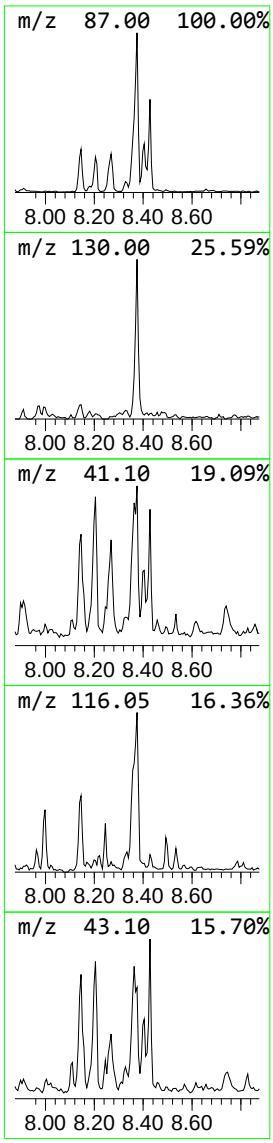
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Heptanoic acid, 2-propyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.375	6.65 ng	454044	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	72
2	Thiophane, propyl-	130	C7H14S	001551-34-4	59
3	2-[2-[2-[2-(2-Butoxyethoxy)ethox...	336	C16H32O7	1000351-94-0	59
4	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	59
5	Thiophene, 2-butyltetrahydro-	144	C8H16S	001613-49-6	42





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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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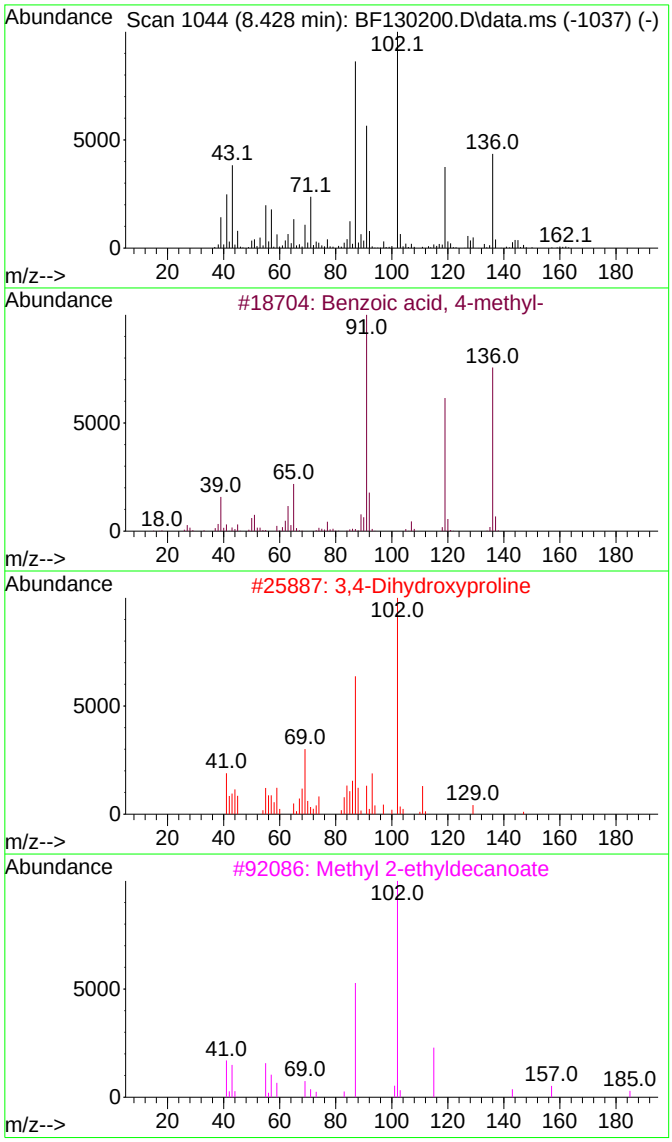
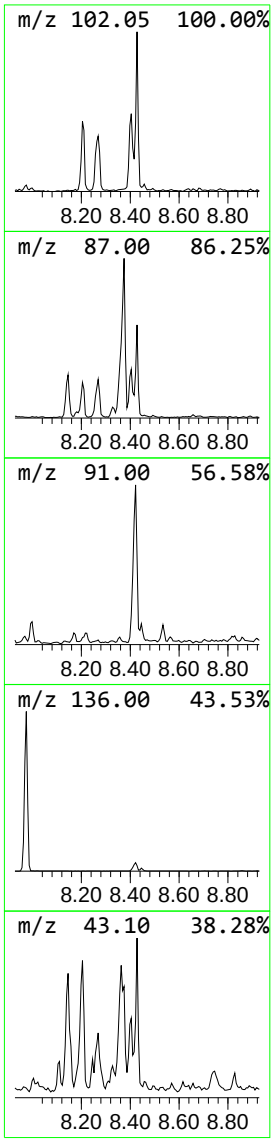
Peak Number 18 Benzoic acid, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	8.05 ng	549429	Naphthalene-d8	7.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	53
2	3,4-Dihydroxyproline	147	C5H9NO4	1000132-90-7	50
3	Methyl 2-ethyldecanoate	214	C13H26O2	020483-47-0	25
4	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	15
5	l-Alanine, N-methoxycarbonyl-, o...	399	C23H45NO4	1000313-38-6	14





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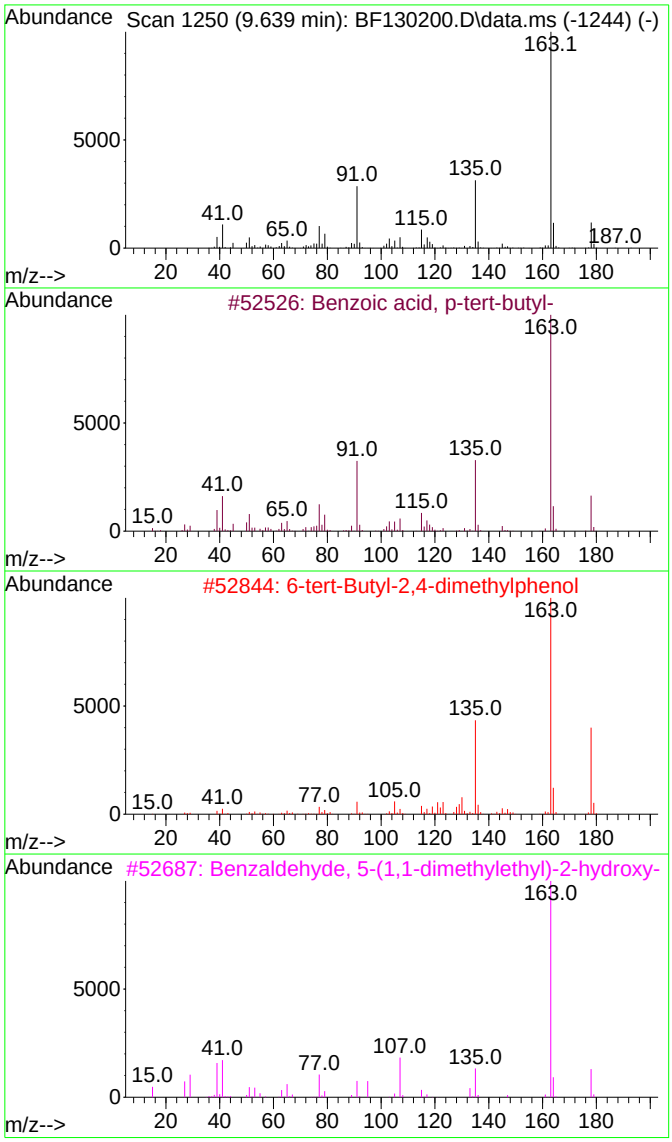
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

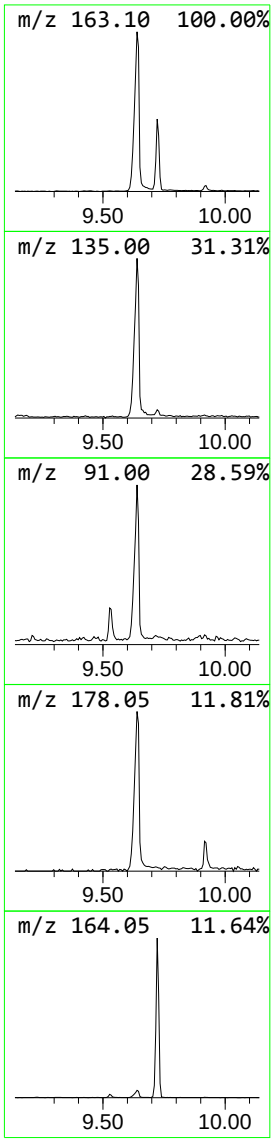
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 Benzoic acid, p-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.639	9.08 ng	664694	Acenaphthene-d10	9.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
3	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	72
4	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	60
5	2-tert-Butyl-4-ethylphenol, O-is...	264	C16H24O3	1000487-42-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

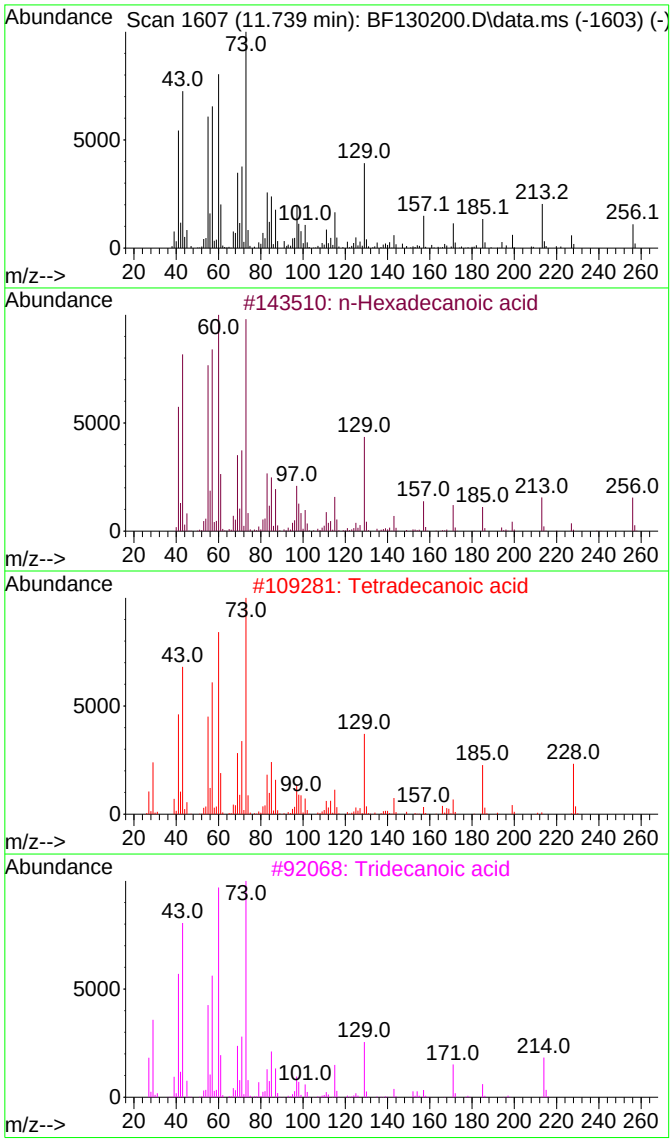
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

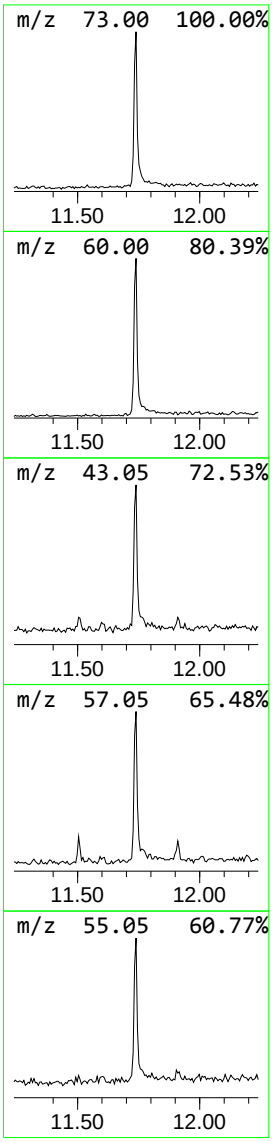
****

Peak Number 20 n-Hexadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	3.39 ng	217344	Phenanthrene-d10	11.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090922\
Data File : BF130200.D
Acq On : 09 Sep 2022 18:03
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.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
Pentane, 2,3,4-...	3.222	3.5	ng	139395	1	6.693	797101	20.0
Di-sec-Butyl ether	4.152	6.4	ng	255091	1	6.693	797101	20.0
3-Pentanol, 3-e...	4.240	4.8	ng	189503	1	6.693	797101	20.0
1,4-Hexadiene, ...	4.393	6.0	ng	238146	1	6.693	797101	20.0
2-Pentanone, 4-...	4.875	3.7	ng	147659	1	6.693	797101	20.0
Benzene, propyl-	6.151	7.9	ng	314157	1	6.693	797101	20.0
Benzene, (2-met...	6.634	4.3	ng	170864	1	6.693	797101	20.0
Indane	6.875	35.8	ng	1427310	1	6.693	797101	20.0
Benzene, 1,2-di...	7.034	4.4	ng	174589	1	6.693	797101	20.0
4,7-Methano-1H-...	7.169	5.8	ng	231119	1	6.693	797101	20.0
Hexanoic acid, ...	7.381	18.9	ng	1291230	2	7.975	1365420	20.0
unknown7.463	7.463	25.8	ng	1760510	2	7.975	1365420	20.0
unknown8.145	8.145	3.8	ng	260130	2	7.975	1365420	20.0
unknown8.204	8.204	6.6	ng	453176	2	7.975	1365420	20.0
Butanoic acid, ...	8.269	4.0	ng	274077	2	7.975	1365420	20.0
Heptanoic acid,...	8.375	6.7	ng	454044	2	7.975	1365420	20.0
Benzoic acid, 4...	8.428	8.1	ng	549429	2	7.975	1365420	20.0
Benzoic acid, p...	9.639	9.1	ng	664694	3	9.722	1464650	20.0
n-Hexadecanoic ...	11.739	3.4	ng	217344	4	11.204	1283390	20.0