LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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: BF130214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.416	15	22	30	rVB2	42822	96857	3.06%	0.349%
2	2.622	51	57	65	rBV5	19254	39046	1.23%	0.141%
3	2.822	87	91	107	rVB5	14472	40357	1.27%	0.145%
4	3.010	119	123	136	rVB4	21192	48925	1.55%	0.176%
5	3.199	141	155	161	rBV4	49464	138186	4.36%	0.497%
6	3.363	171	183	190	rBV2	57127	140978	4.45%	0.507%
7	3.510	202	208	214	rBV3	27168	54330	1.72%	0.196%
8	3.581	215	220	224	rBV2	26336	47124	1.49%	0.170%
9	3.693	232	239	243	rBV	43529	70114	2.21%	0.252%
10	3.910	271	276	282	rVB5	27908	50113	1.58%	0.180%
11	4.140	306	315	325	rVB	199103	298416	9.42%	1.074%
12	4.228	325	330	334	rBV	196629	226125	7.14%	0.814%
13	4.381	348	356	364	rBV	167938	218973	6.92%	0.788%
14	4.646	395	401	403	rBV	53492	73904	2.33%	0.266%
15	4.669	403	405	410	rVB	37312	45539	1.44%	0.164%
16	4.863	434	438	445	rVV	131228	145608	4.60%	0.524%
17	4.934	446	450	455	rVB	38763	41227	1.30%	0.148%
18	5.281	505	509	513	rVB	1700003	1639750	51.78%	5.901%
19	5.698	575	580	584	rBV3	32624	48613	1.54%	0.175%
20	5.851	601	606	609	rBV	406664	364338	11.51%	1.311%
21	5.998	626	631	635	rBV5	24327	40594	1.28%	0.146%
22	6.145	653	656	659	rVB	347421	293652	9.27%	1.057%
23	6.310	680	684	691	rVB	1190590	1044571	32.99%	3.759%
24	6.369	691	694	696	rBV	83313	62885	1.99%	0.226%
25	6.628	732	738	740	rBV	113258	134272	4.24%	0.483%
26	6.687	744	748	751	rBV	1015476	776187	24.51%	2.793%
27	6.810	766	769	771	rBV	70348	52155	1.65%	0.188%
28	6.869	775	779	782	rVB	948950	860039	27.16%	3.095%
29	6.939	788	791	793	rBV	79912	64066	2.02%	0.231%
30	7.010	800	803	804	rBV	42149	41594	1.31%	0.150%
31	7.028	804	806	811	rVB	136581	105191	3.32%	0.379%
32	7.081	811	815	817	rBV	45787	44075	1.39%	0.159%
33	7.163	825	829	832	rVB	212118	173899	5.49%	0.626%
34	7.222	833	839	840	rBV	60853	65718	2.08%	0.236%
35	7.251	840	844	847	rVB2	2871565	2610383	82.44%	9.394%
36	7.381	852	866	867	rBV3	450396	1020088	32.21%	3.671%

LSC Area Percent Report

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Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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	7.422	867	873	874	rBV	311052	474754	14.99%	1.708%
38	7.457	874	879	882	rBV2	588153	1177610	37.19%	4.238%
39	7.516	884	889	890	rBV	570200	789103	24.92%	2.840%
40	7.563	891	897	898	rBV	744930	1325915	41.87%	4.771%
41	7.657	909	913	917	rVB2	83327	98034	3.10%	0.353%
42	7.704	917	921	926	rVB3	52751	58234	1.84%	0.210%
43	7.810	931	939	942	rVB	405141	674076	21.29%	2.426%
44	7.969	962	966	968	rBV	776726	696620	22.00%	2.507%
45	7.986	968	969	972	rVB2	87666	68238	2.15%	0.246%
46	8.128	990	993	997	rBV	108797	115198	3.64%	0.415%
47	8.186	997	1003	1006	rBV5	121487	173442	5.48%	0.624%
48	8.257	1011	1015	1019	rVB4	85397	115674	3.65%	0.416%
49	8.357	1027	1032	1035	rBV2	131917	199766	6.31%	0.719%
50	8.410	1035	1041	1044	rVV3	159130	241422	7.62%	0.869%
51	8.528	1057	1061	1064	rBV	87768	68663	2.17%	0.247%
52	8.775	1098	1103	1105	rBV3	38170	48397	1.53%	0.174%
53	9.045	1144	1149	1152	rBV	4028682	3166581	100.00%	11.395%
54	9.522	1227	1230	1235	rVB3	48904	56898	1.80%	0.205%
55	9.628	1243	1248	1251	rBV	251882	276849	8.74%	0.996%
56	9.716	1257	1263	1266	rBV	898655	715912	22.61%	2.576%
57	9.745	1266	1268	1275	rVB	56703	56048	1.77%	0.202%
58	9.857	1284	1287	1293	rBV	95007	99271	3.13%	0.357%
59	10.080	1322	1325	1328	rBV	105840	90067	2.84%	0.324%
60	10.504	1392	1397	1408	rBV	1839657	1847554	58.35%	6.649%
61	11.192	1511	1514	1518	rBV	612963	559063	17.66%	2.012%
62	11.733	1602	1606	1611	rBV	106152	110474	3.49%	0.398%
63	12.404	1716	1720	1730	rBV	40618	49085	1.55%	0.177%
64	12.516	1736	1739	1745	rBV	53283	57641	1.82%	0.207%
65	12.780	1780	1784	1788	rBV	2312890	2123998	67.08%	7.644%
66	13.827	1958	1962	1965	rBV	489822	474895	15.00%	1.709%
67	15.221	2195	2199	2204	rBV	494619	560852	17.71%	2.018%

Sum of corrected areas: 27788226

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
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Acq On : 12 Sep 2022 20:08
Operator : CG\JU
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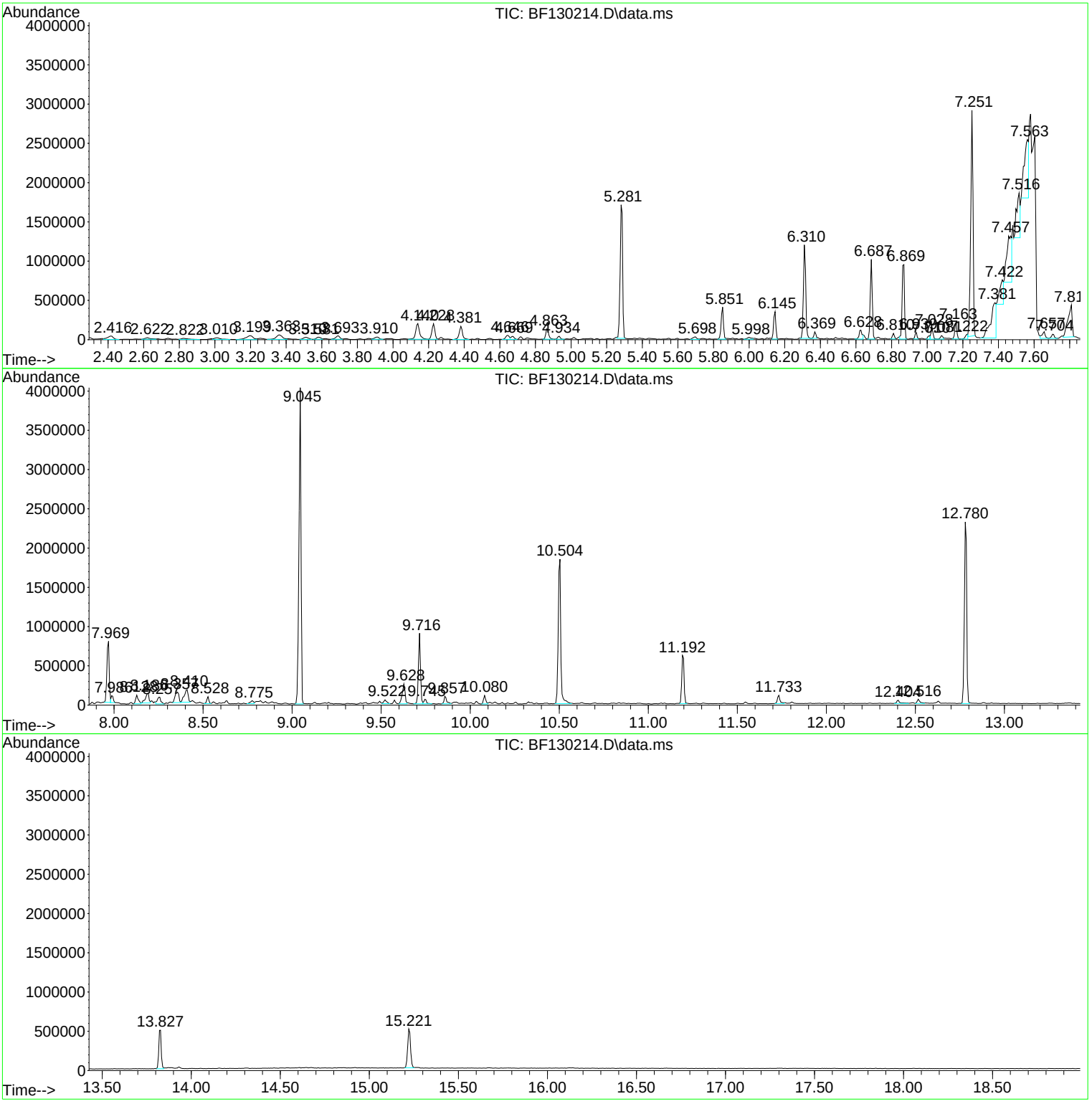
Misc :
ALS Vial : 11 Sample Multiplier: 1

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

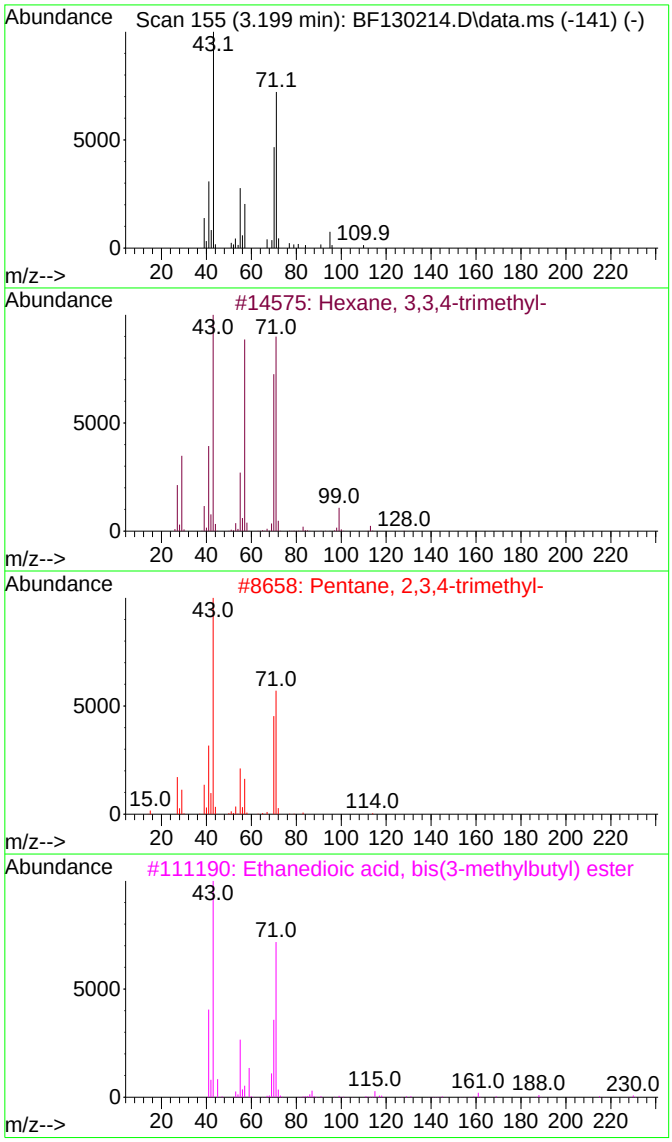
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

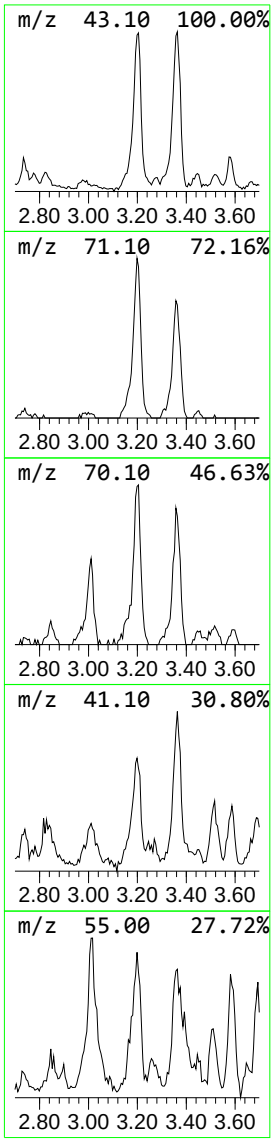
****

Peak Number 1 Hexane, 3,3,4-trimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.199	3.56 ng	138186	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	72
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	72
3	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	56
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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

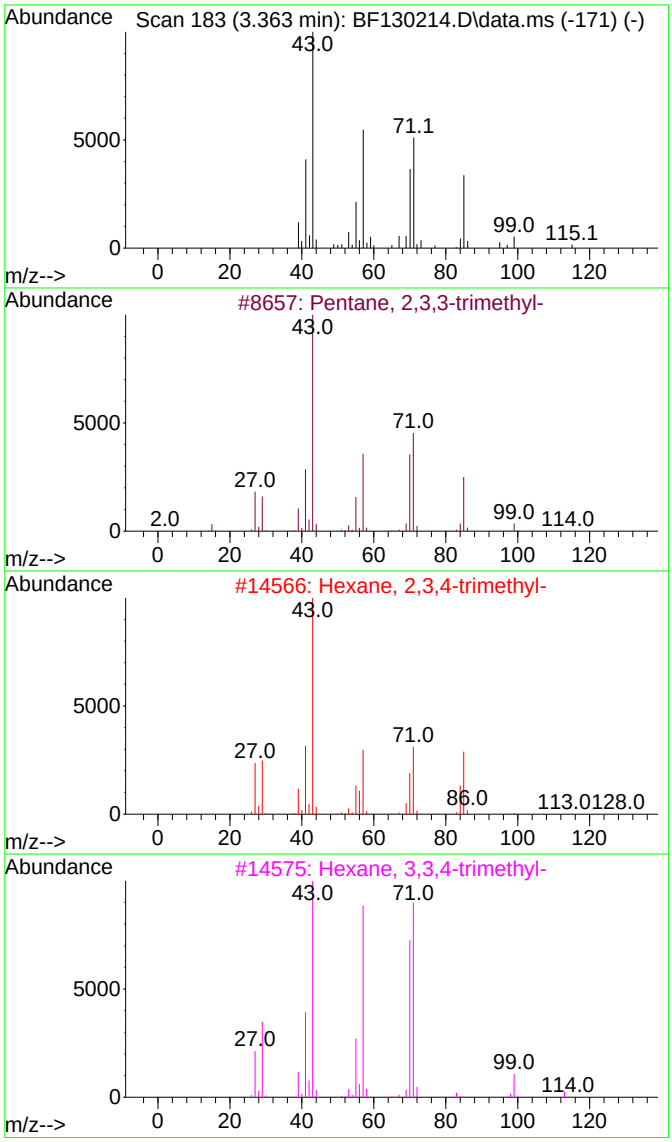
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

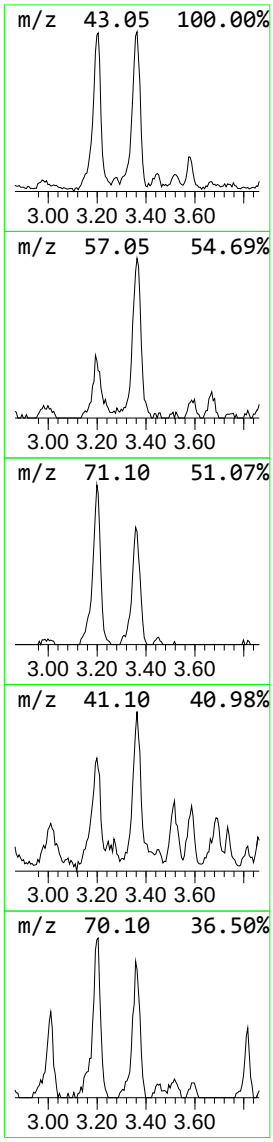
****

Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	3.63 ng	140978	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	47
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	45
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
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Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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

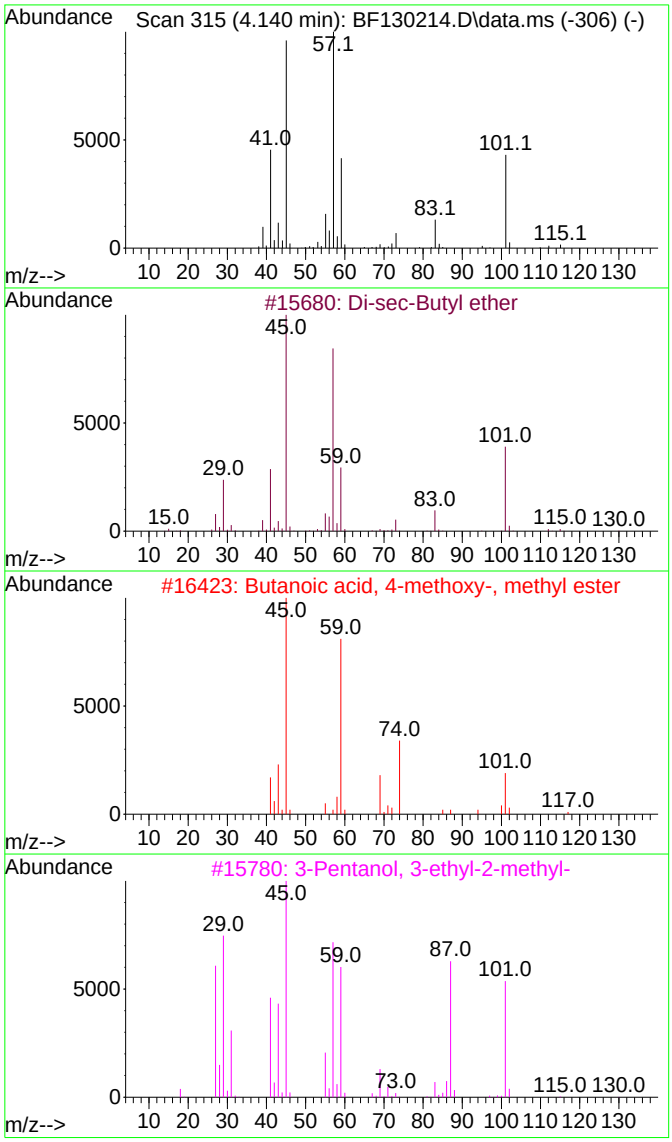
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

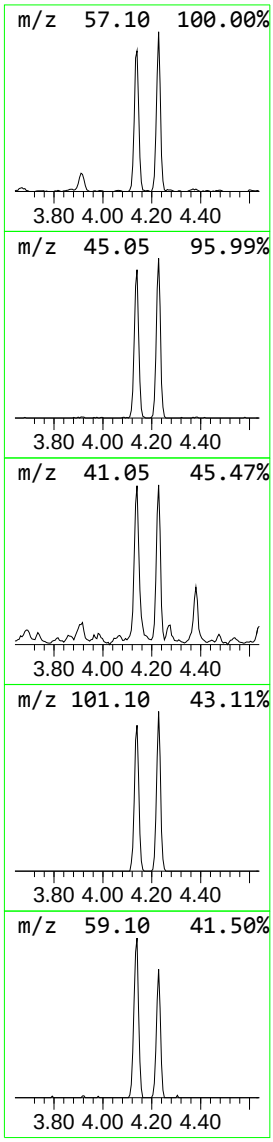
****

Peak Number 3 Di-sec-Butyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.140	7.69 ng	298416	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	64
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	56
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5	Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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

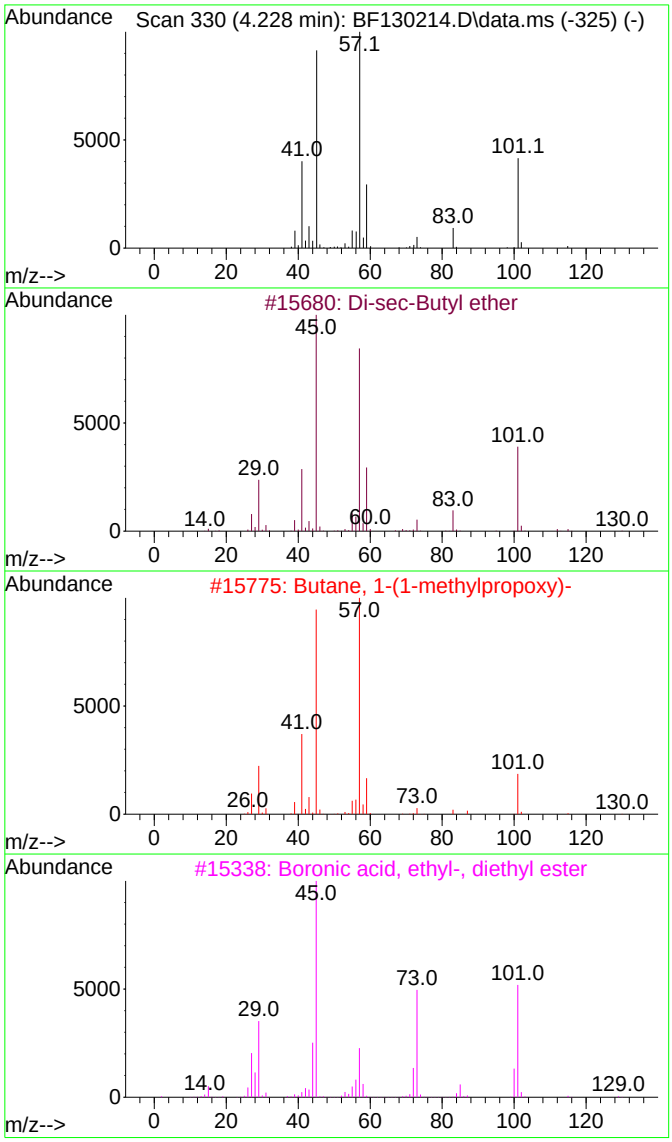
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

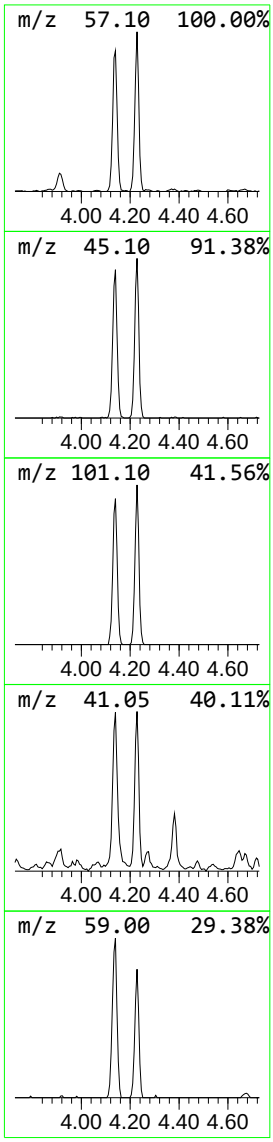
****

Peak Number 4 Butane, 1-(1-methylpropoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.228	5.83 ng	226125	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	42
4	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	38
5	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

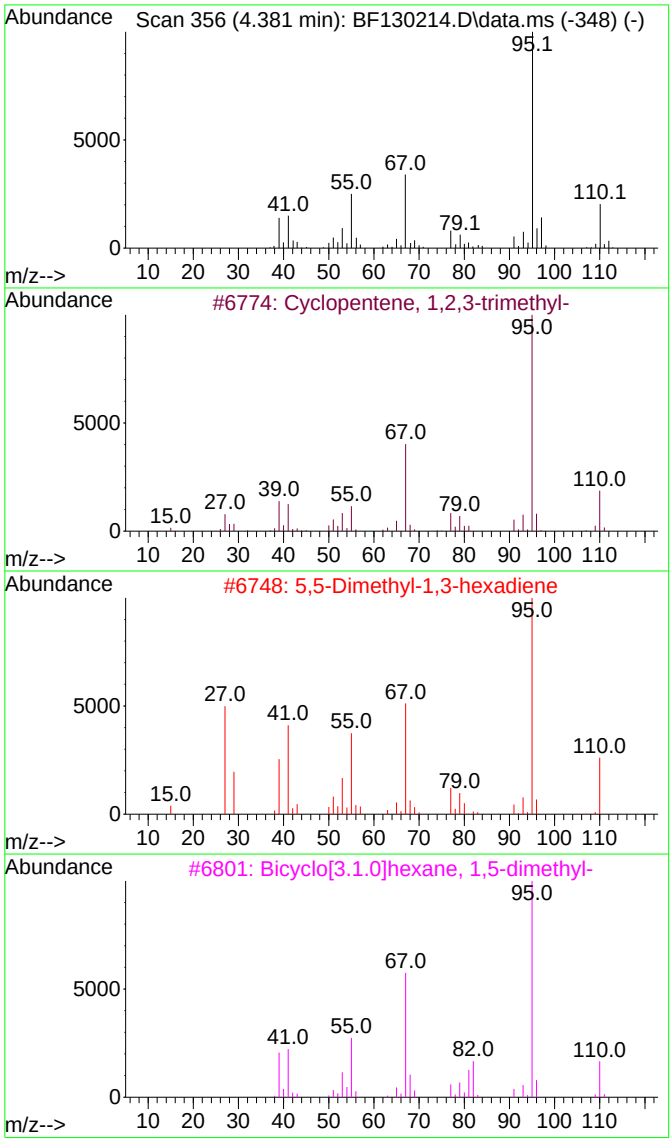
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

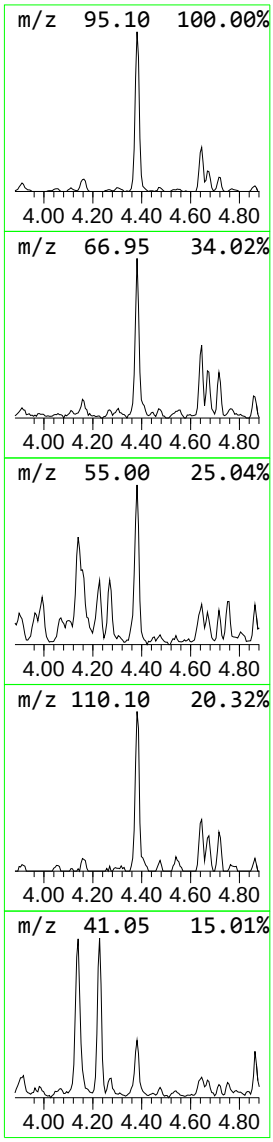
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.381	5.64 ng	218973	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	93
2	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	87
3	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	86
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	83
5	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

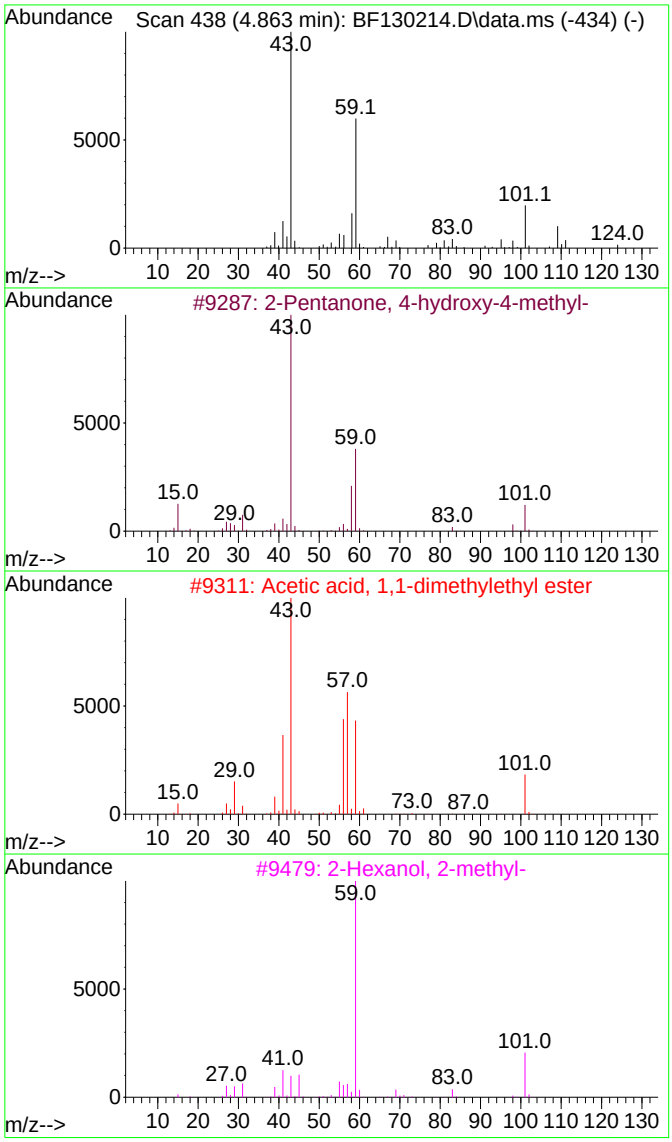
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

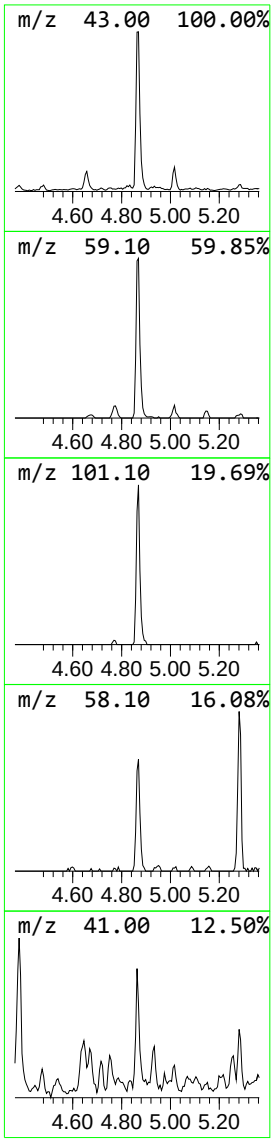
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	3.75 ng	145608	1,4-Dichlorobenzene-d4	6.687

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	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	12
5	2,3-Dimethyl-4-penten-2-ol	114	C7H14O	019781-52-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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

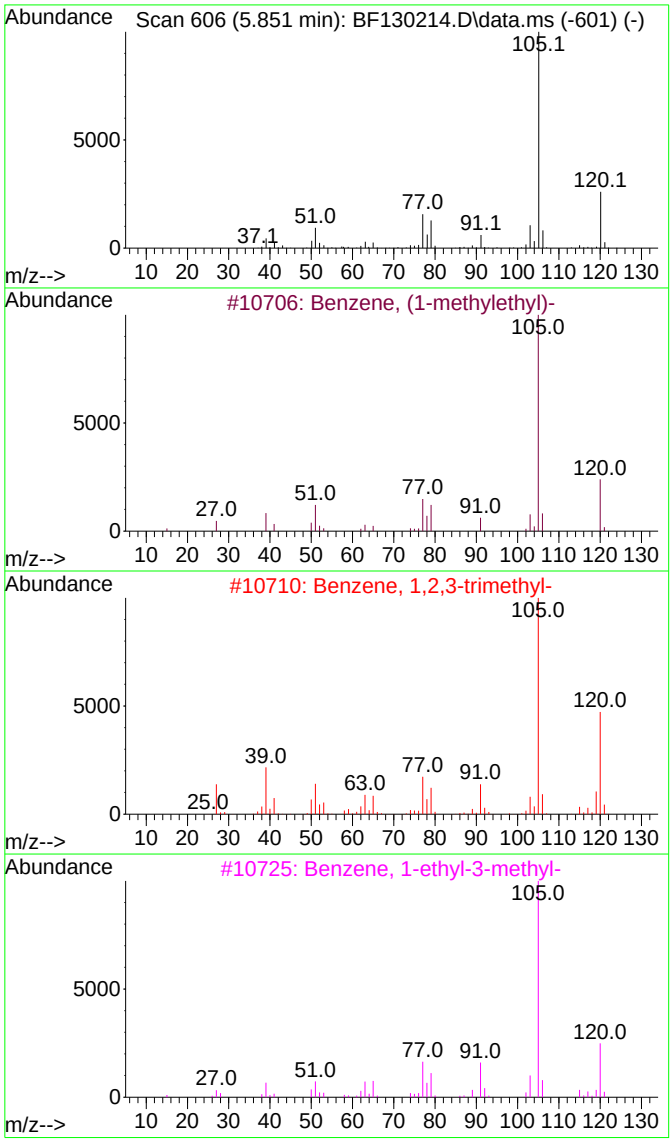
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

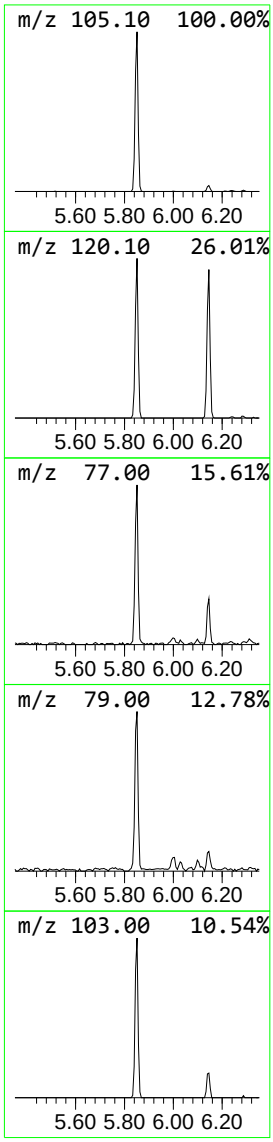
****

Peak Number 7 Benzene, (1-methylethyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	9.39 ng	364338	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	95
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	83
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	83
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	78





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Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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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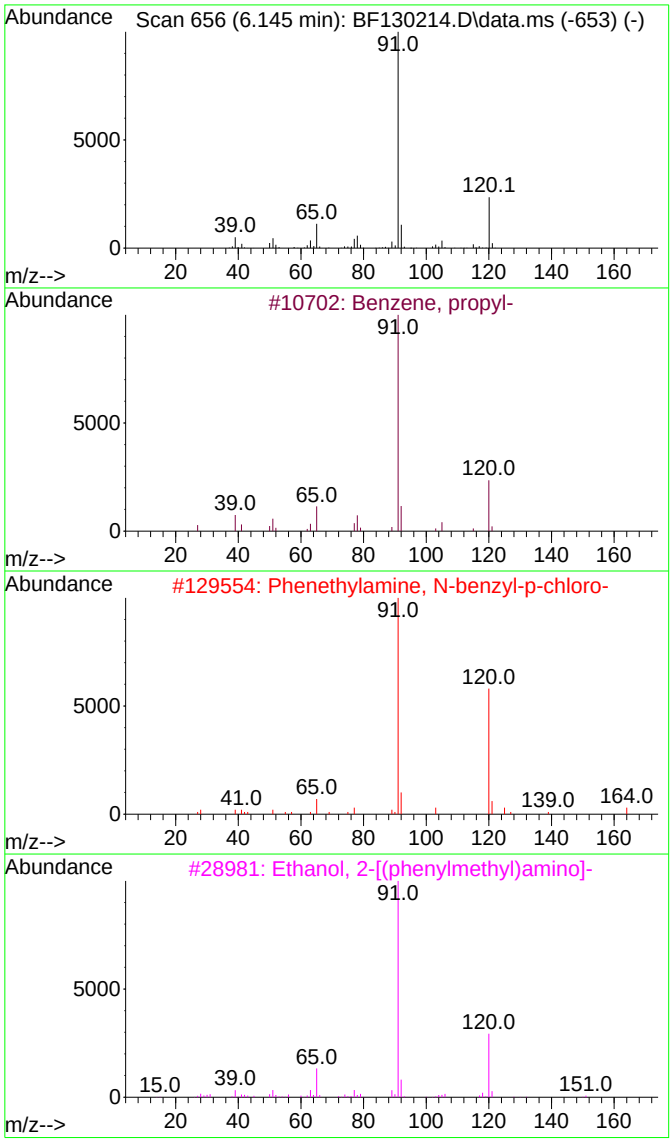
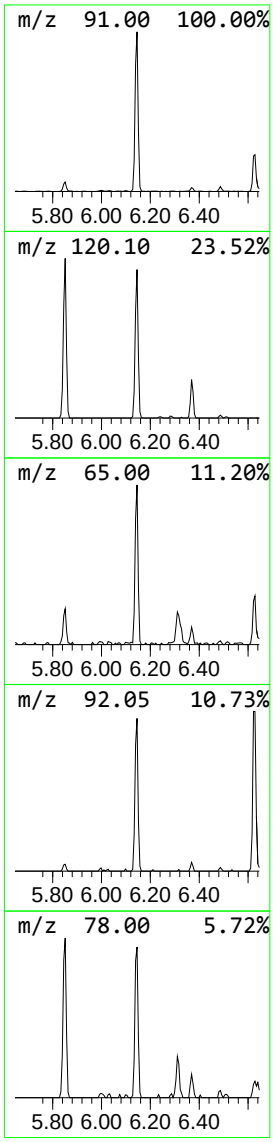
Peak Number 8 Benzene, propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.145	7.57 ng	293652	1,4-Dichlorobenzene-d4	6.687

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	Ethanol, 2-[(phenylmethyl)amino]-	151	C9H13NO	000104-63-2	72
4	1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	64
5	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	59





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Misc :
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BNA_F
ClientSampleId :
DUP090822

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

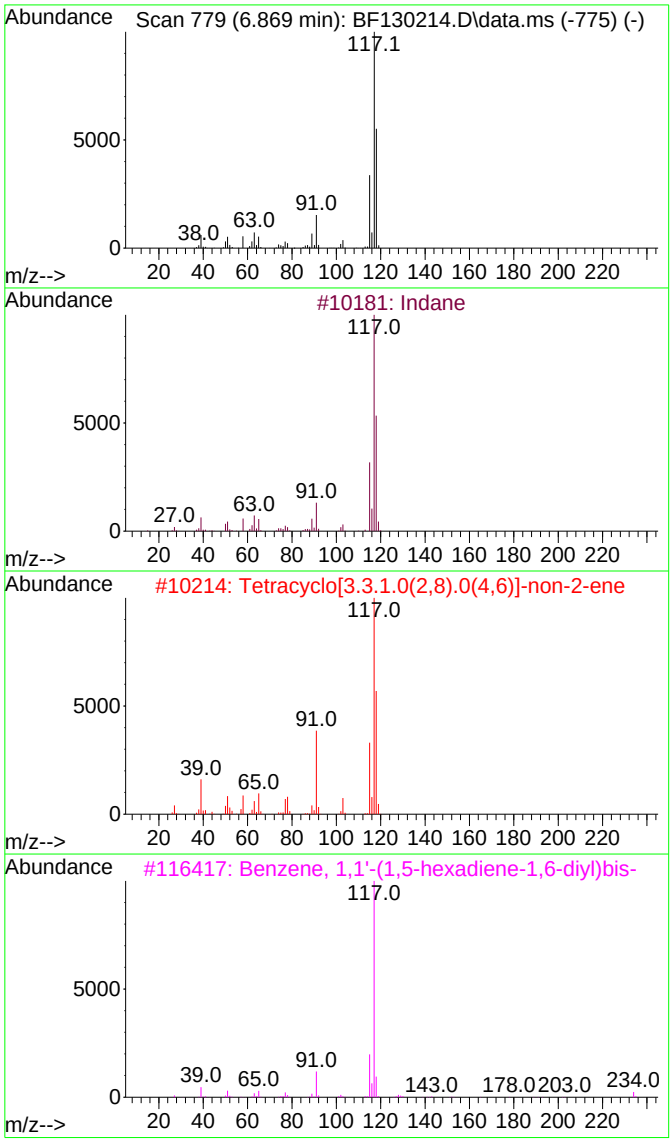
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

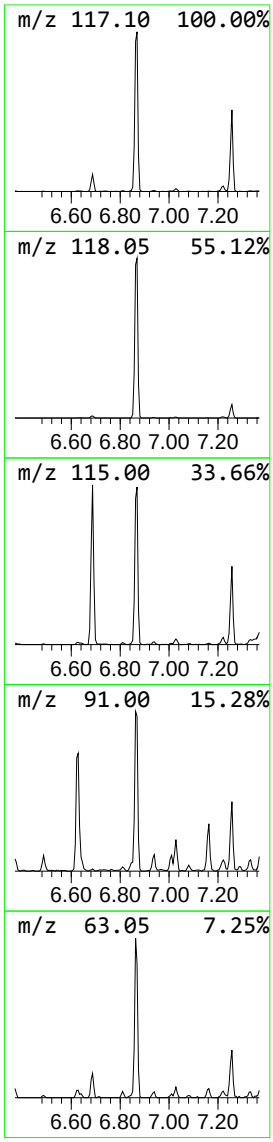
****

Peak Number 9 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.869	22.16 ng	860039	1,4-Dichlorobenzene-d4	6.687

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	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
4	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53





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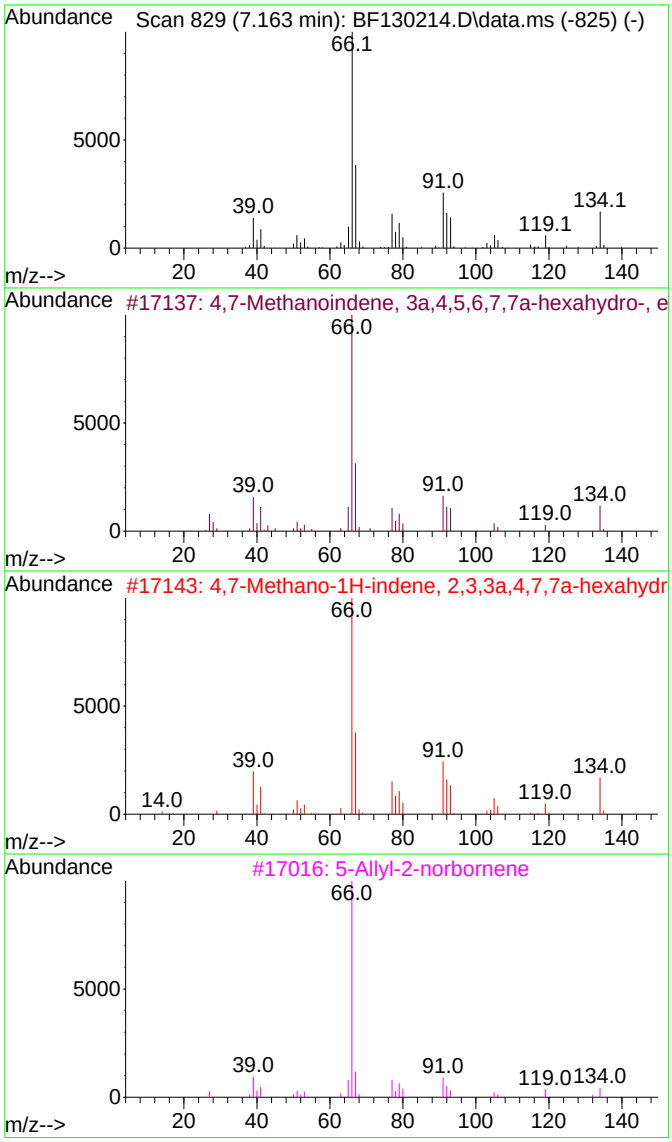
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

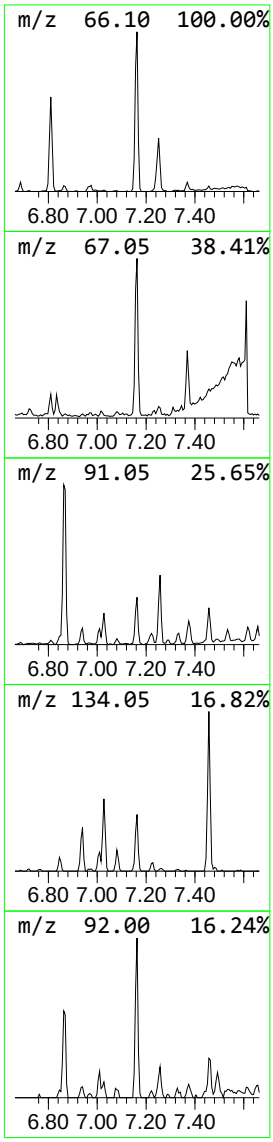
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 4,7-Methanoindene, 3a,4,5,6... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	4.48 ng	173899	1,4-Dichlorobenzene-d4	6.687

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methanoindene, 3a,4,5,6,7,7a...	134	C10H14	002825-86-7	96
2	4,7-Methano-1H-indene, 2,3,3a,4,...	134	C10H14	002826-19-9	94
3	5-Allyl-2-norbornene	134	C10H14	031663-53-3	90
4	3a,4,5,6,7,7a-Hexahydro-4,7-meth...	134	C10H14	004488-57-7	90
5	5-Norbornane-2-carboxaldehyde	122	C8H10O	005453-80-5	72





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ALS Vial : 11 Sample Multiplier: 1

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

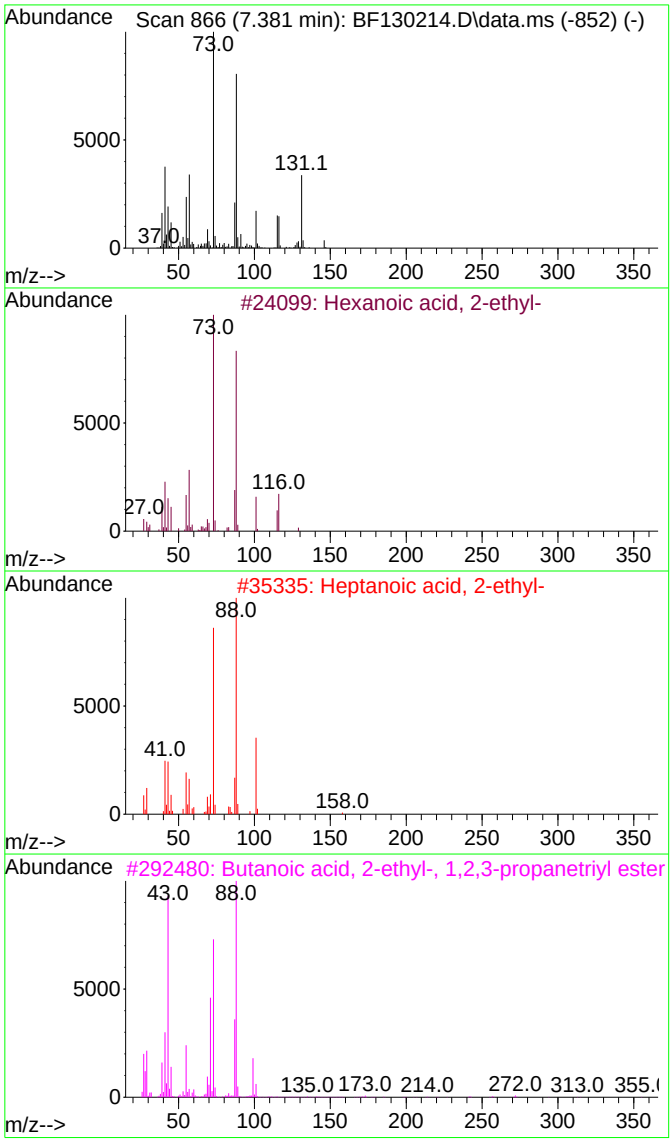
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

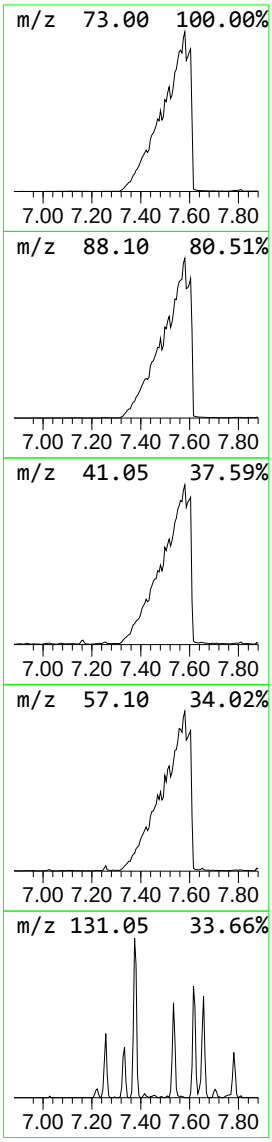
****

Peak Number 11 Heptanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.381	29.29 ng	1020090	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	50
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	47
4	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
5	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	43





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Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP090822

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

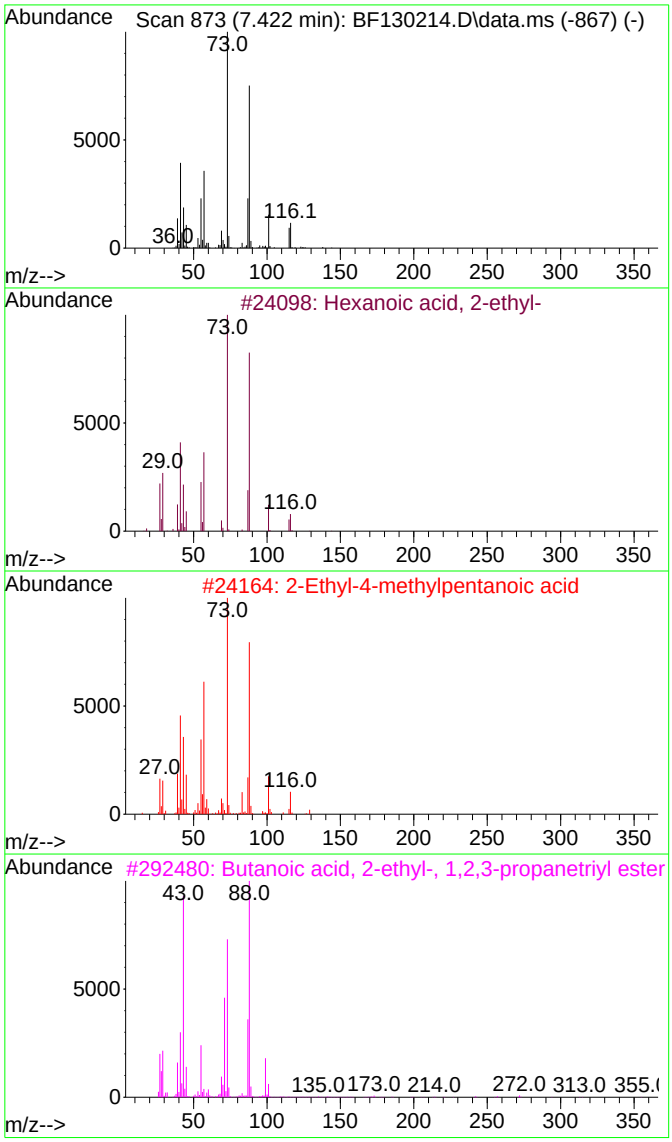
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

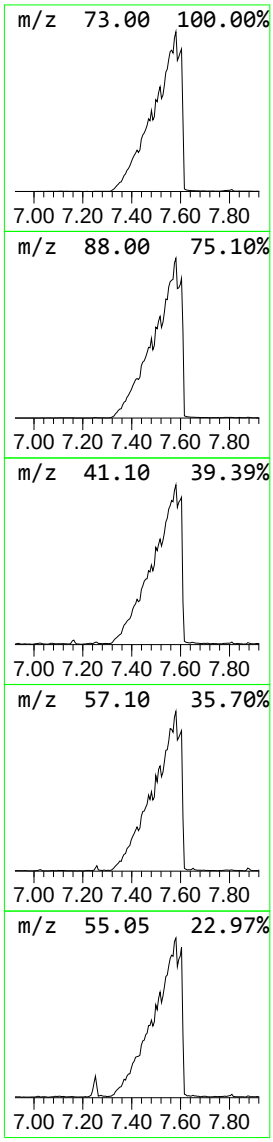
****

Peak Number 12 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.422	13.63 ng	474754	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	64
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	45





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Misc :
ALS Vial : 11 Sample Multiplier: 1

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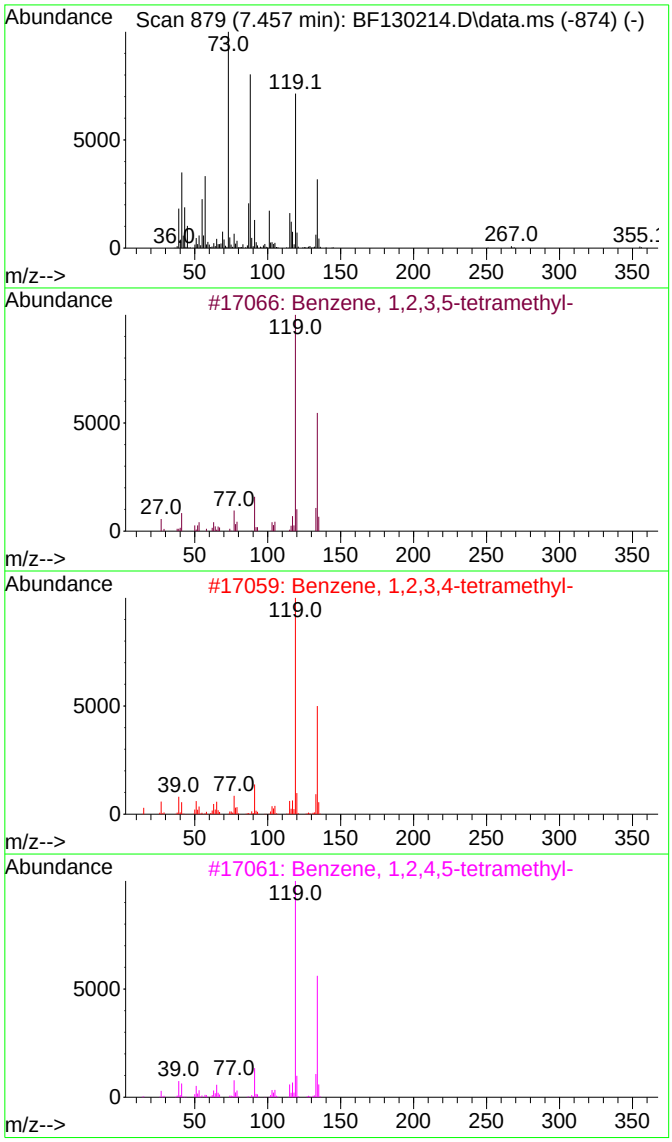
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

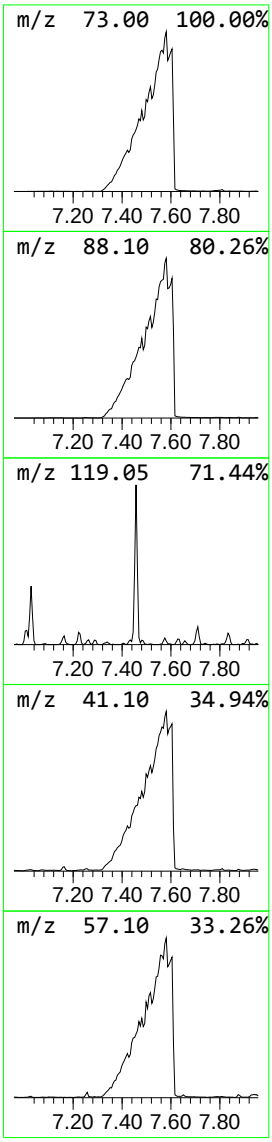
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.457	33.81 ng	1177610	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	70
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	38
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	38
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	38
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	38





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Sample : N4549-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP090822

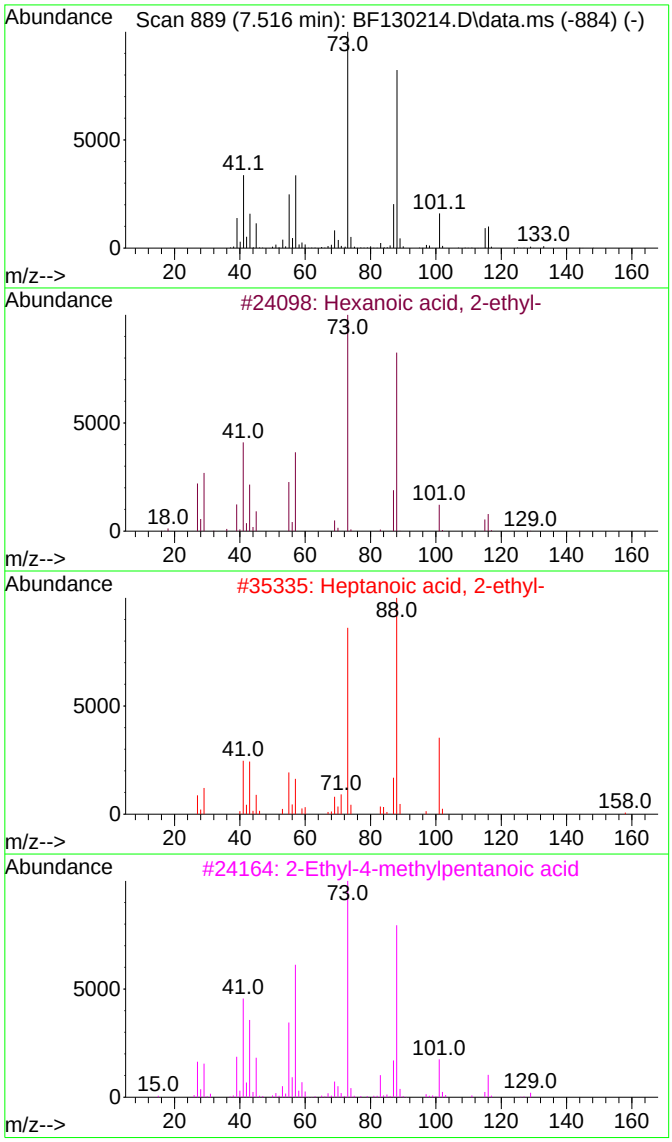
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

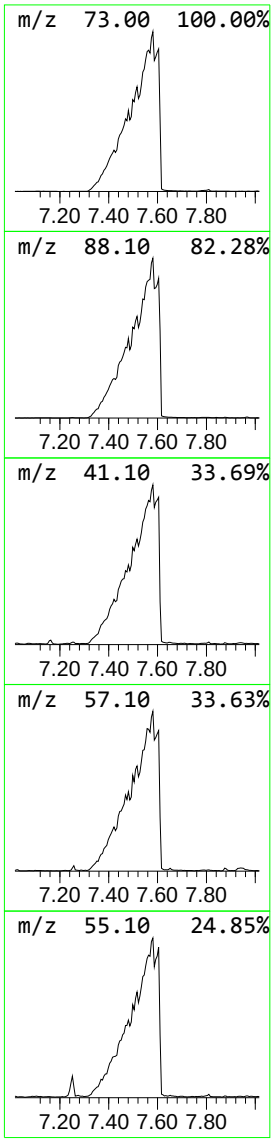
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2-Ethyl-4-methylpentanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.516	22.66 ng	789103	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





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ALS Vial : 11 Sample Multiplier: 1

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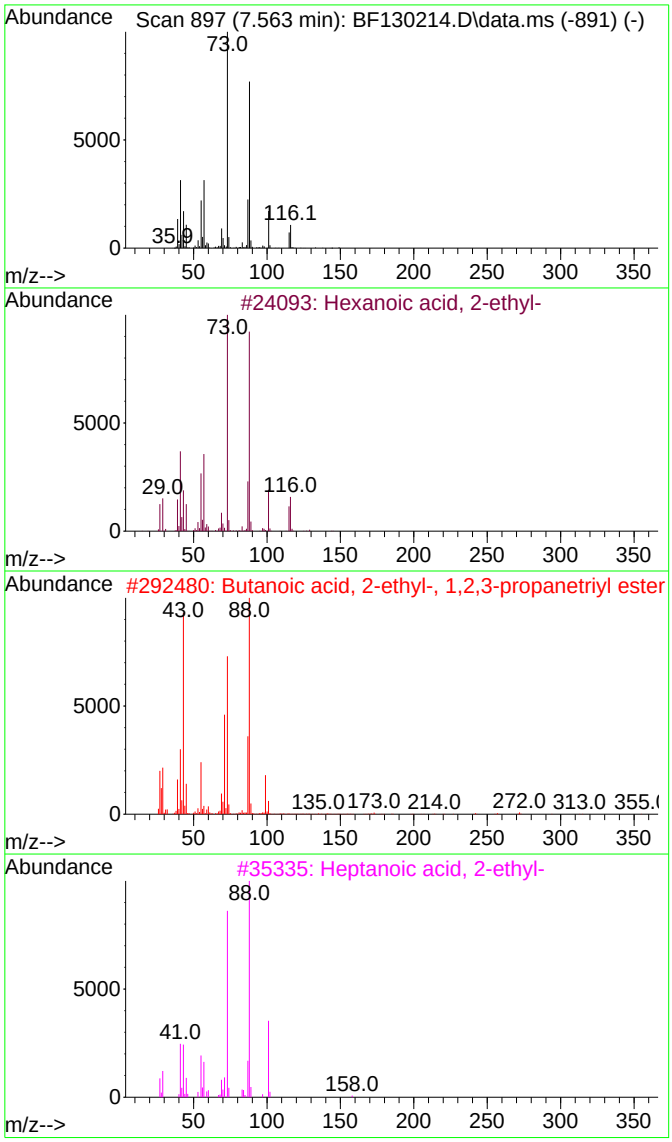
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

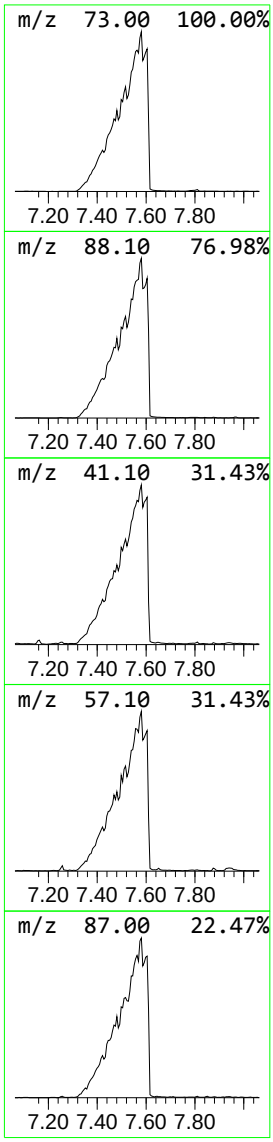
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Butanoic acid, 2-ethyl-, 1,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	38.07 ng	1325920	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	50
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	40





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ALS Vial : 11 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

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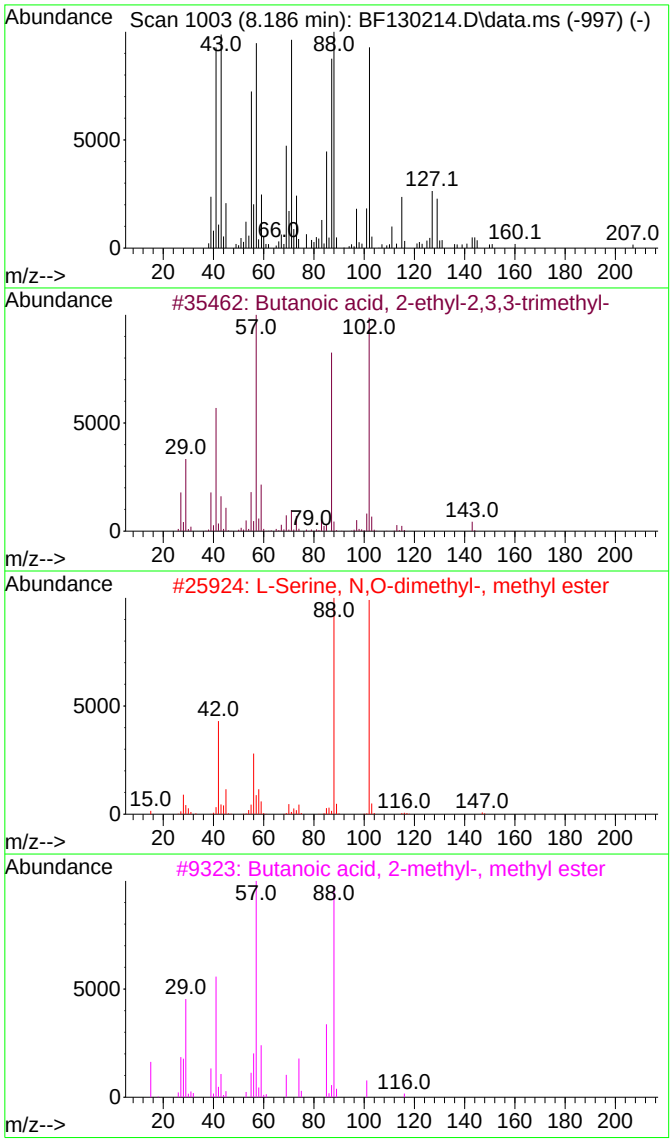
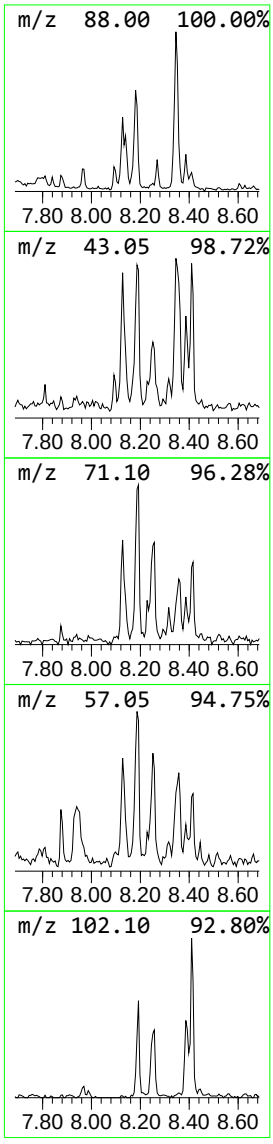
Peak Number 16 unknown8.186 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.186	4.98 ng	173442	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-2,3,3-tri...	158	C9H18O2	038541-67-2	27
2	L-Serine, N,O-dimethyl-, methyl ...	147	C6H13NO3	1000452-63-9	22
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	20
4	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	18
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	14





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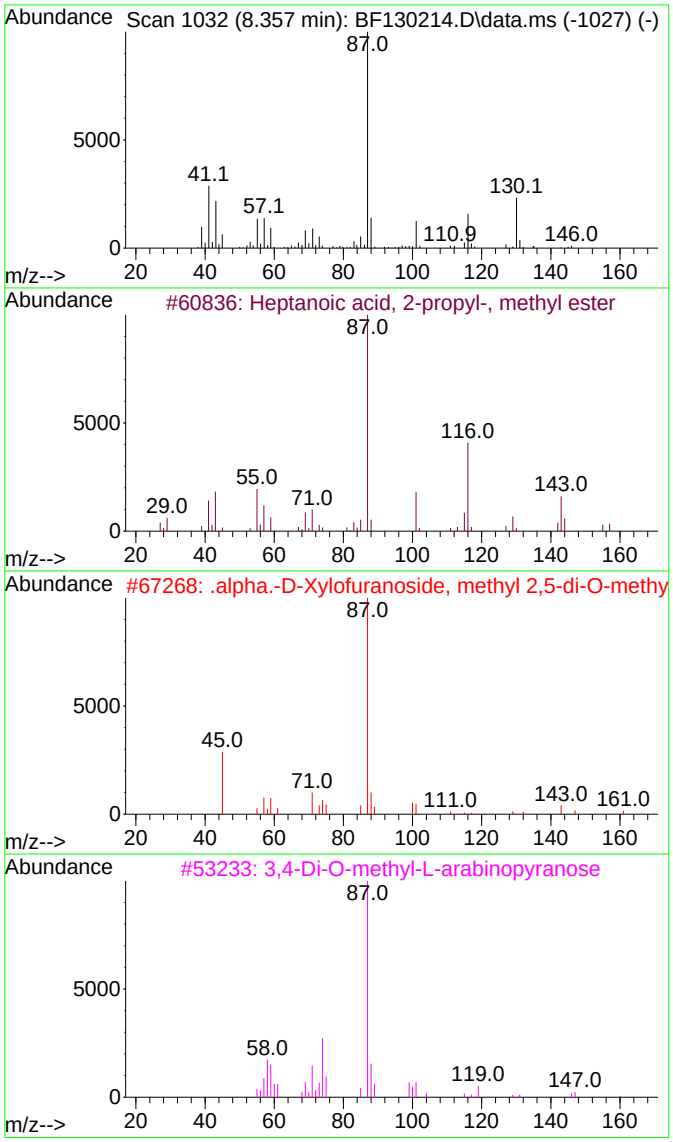
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

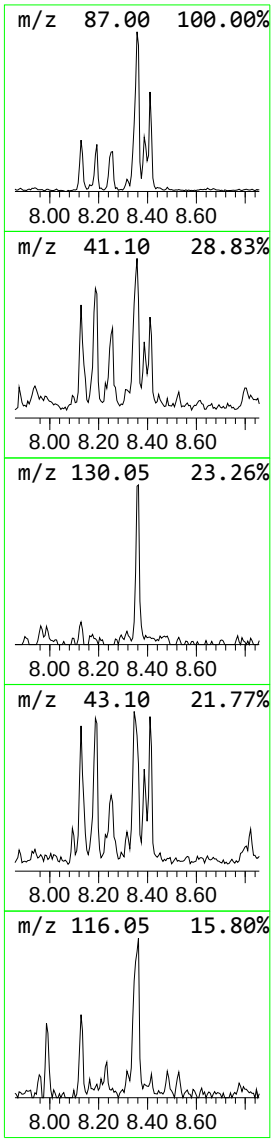
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Heptanoic acid, 2-propyl-, ... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	5.74 ng	199766	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	59
2	.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	53
3	3,4-Di-O-methyl-L-arabinopyranose	178	C7H14O5	086049-20-9	42
4	Borinic acid, diethylthio-, meth...	116	C5H13BS	092276-84-1	38
5	2-[2-[2-[2-[2-[2-(2-Acetyloxyeth...	410	C18H34O10	1000351-90-7	38





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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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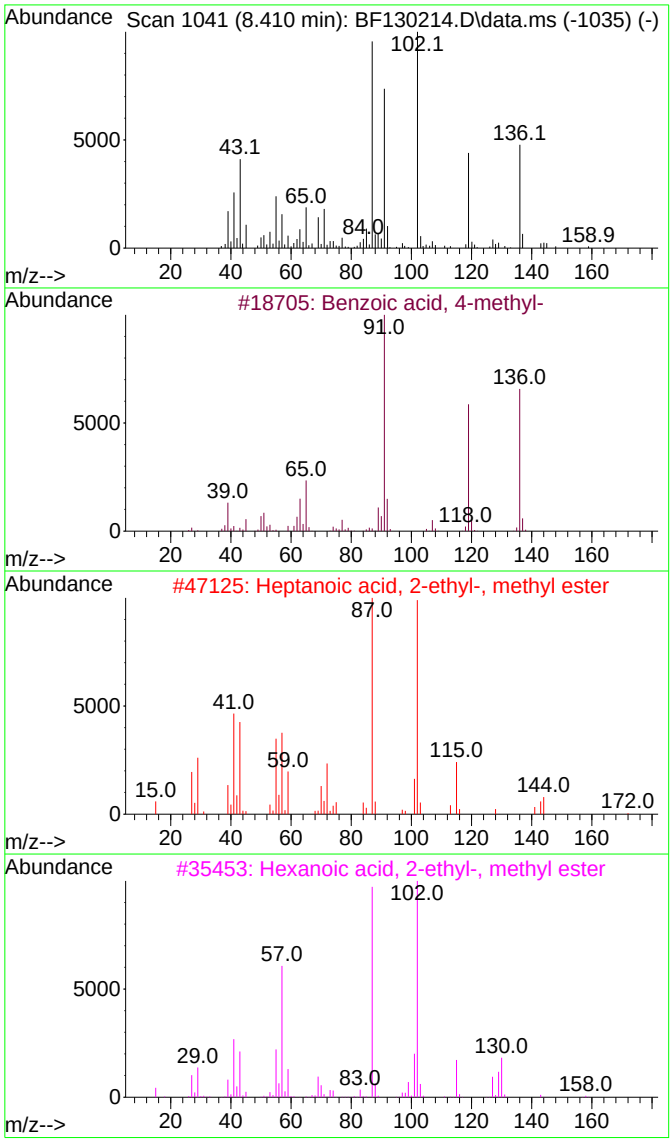
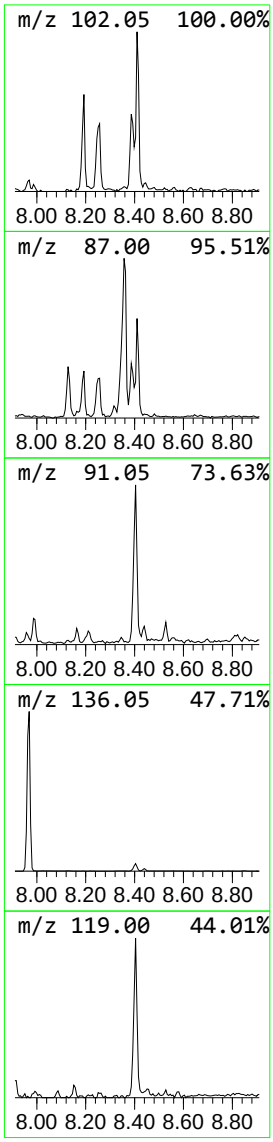
Peak Number 18 Benzoic acid, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.410	6.93 ng	241422	Naphthalene-d8	7.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	93
2	Heptanoic acid, 2-ethyl-, methyl...	172	C10H20O2	000816-63-7	43
3	Hexanoic acid, 2-ethyl-, methyl ...	158	C9H18O2	000816-19-3	37
4	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	30
5	l-Alanine, N-methoxycarbonyl-, h...	385	C22H43NO4	1000313-38-5	14





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Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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

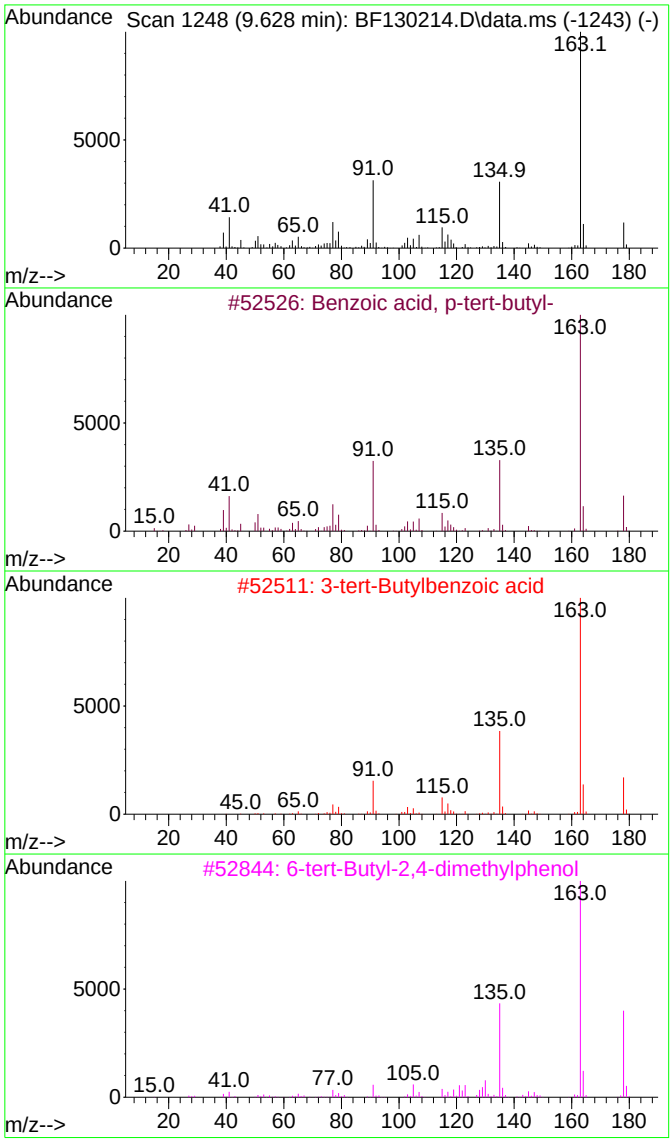
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

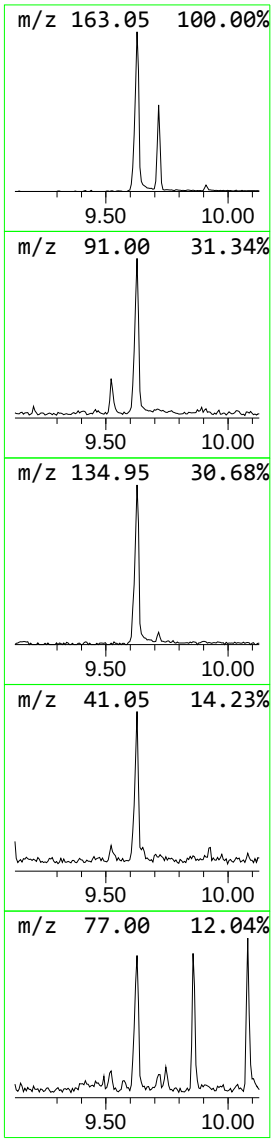
****

Peak Number 19 Benzoic acid, p-tert-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.628	7.73 ng	276849	Acenaphthene-d10	9.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	90
3	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
4	2,3,4,5,6-Pentamethylphenol, met...	178	C12H18O	014804-37-6	64
5	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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

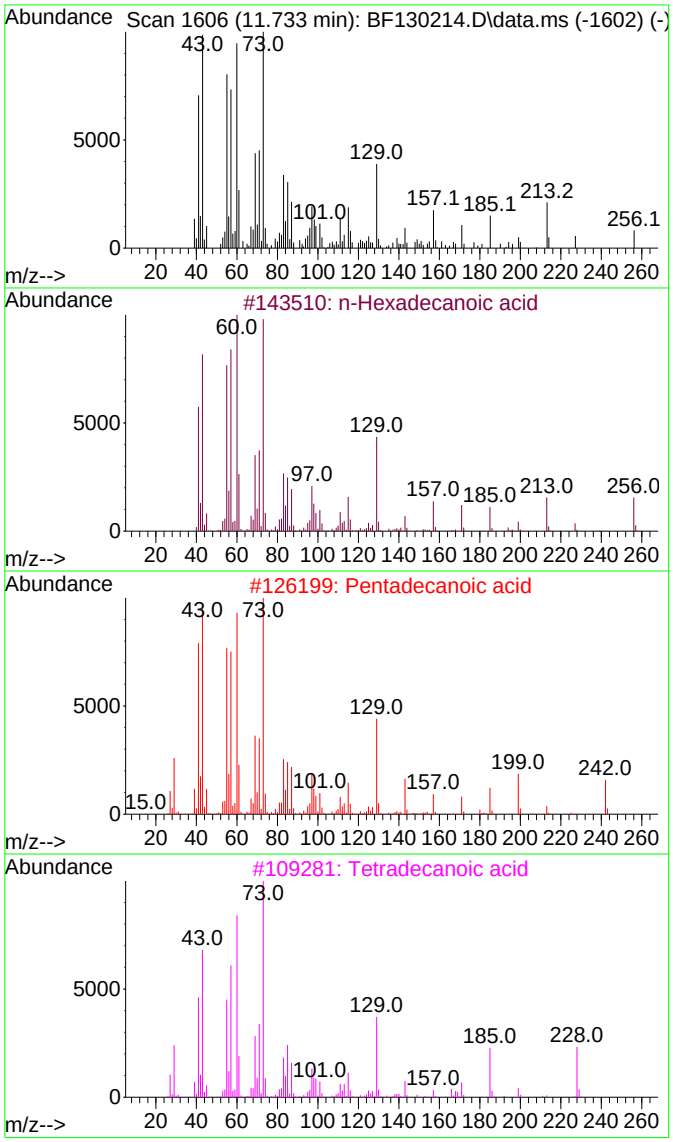
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

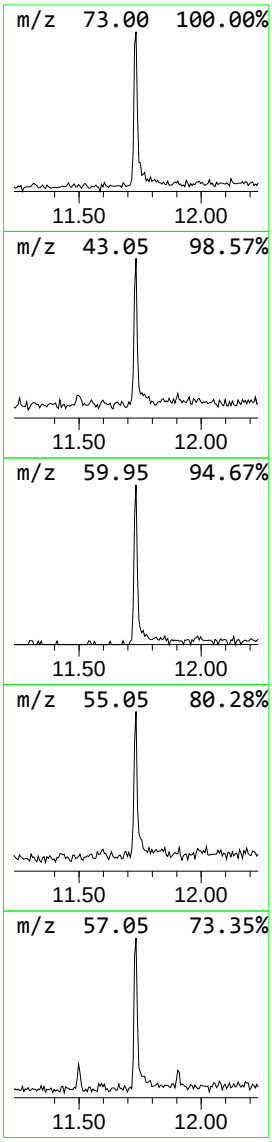
****

Peak Number 20 n-Hexadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.733	3.95 ng	110474	Phenanthrene-d10	11.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091222\
Data File : BF130214.D
Acq On : 12 Sep 2022 20:08
Operator : CG\JU
Sample : N4549-21
Misc :
ALS Vial : 11 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
Hexane, 3,3,4-t...	3.199	3.6	ng	138186	1	6.687	776187	20.0
Pentane, 2,3,3-...	3.363	3.6	ng	140978	1	6.687	776187	20.0
Di-sec-Butyl ether	4.140	7.7	ng	298416	1	6.687	776187	20.0
Butane, 1-(1-me...	4.228	5.8	ng	226125	1	6.687	776187	20.0
Cyclopentene, 1...	4.381	5.6	ng	218973	1	6.687	776187	20.0
2-Pentanone, 4-...	4.863	3.8	ng	145608	1	6.687	776187	20.0
Benzene, (1-met...	5.851	9.4	ng	364338	1	6.687	776187	20.0
Benzene, propyl-	6.145	7.6	ng	293652	1	6.687	776187	20.0
Indane	6.869	22.2	ng	860039	1	6.687	776187	20.0
4,7-Methanoinde...	7.163	4.5	ng	173899	1	6.687	776187	20.0
Heptanoic acid,...	7.381	29.3	ng	1020090	2	7.969	696620	20.0
Hexanoic acid, ...	7.422	13.6	ng	474754	2	7.969	696620	20.0
Benzene, 1,2,3,...	7.457	33.8	ng	1177610	2	7.969	696620	20.0
2-Ethyl-4-methy...	7.516	22.7	ng	789103	2	7.969	696620	20.0
Butanoic acid, ...	7.563	38.1	ng	1325920	2	7.969	696620	20.0
unknown8.186	8.186	5.0	ng	173442	2	7.969	696620	20.0
Heptanoic acid,...	8.357	5.7	ng	199766	2	7.969	696620	20.0
Benzoic acid, 4...	8.410	6.9	ng	241422	2	7.969	696620	20.0
Benzoic acid, p...	9.628	7.7	ng	276849	3	9.716	715912	20.0
n-Hexadecanoic ...	11.733	4.0	ng	110474	4	11.192	559063	20.0