LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
Data File : BF128379.D
Acq On : 20 May 2022 22:35
Operator : CG\JU
Sample : N2943-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-34

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-BF052022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.181	146	152	158	rBV	80841	140456	4.51%	0.691%
2	3.699	234	240	249	rVB6	15312	33981	1.09%	0.167%
3	4.375	350	355	359	rBV	100349	116043	3.73%	0.571%
4	4.463	365	370	375	rVB2	111182	150145	4.82%	0.739%
5	5.334	515	518	525	rVB	85200	88592	2.85%	0.436%
6	5.481	539	543	553	rVB	1205554	1213471	38.99%	5.973%
7	6.487	711	714	721	rBV	865226	837911	26.92%	4.124%
8	6.534	721	722	731	rVB2	34568	39625	1.27%	0.195%
9	6.675	743	746	755	rBV4	48561	101806	3.27%	0.501%
10	6.857	773	777	783	rBV	648631	564453	18.13%	2.778%
11	6.916	783	787	793	rVB2	54989	57829	1.86%	0.285%
12	7.034	800	807	810	rBV	374743	413078	13.27%	2.033%
13	7.116	814	821	828	rVV3	176798	376096	12.08%	1.851%
14	7.187	831	833	839	rVB	63356	58281	1.87%	0.287%
15	7.245	839	843	849	rBV2	37674	42563	1.37%	0.210%
16	7.387	857	867	868	rBV2	95630	115490	3.71%	0.568%
17	7.428	868	874	877	rVV	2096088	2508124	80.58%	12.345%
18	7.475	879	882	890	rVV2	370288	635418	20.41%	3.128%
19	7.557	890	896	900	rVV3	187161	282711	9.08%	1.392%
20	7.622	904	907	909	rVV	67067	67738	2.18%	0.333%
21	7.645	909	911	915	rVV	53603	44037	1.41%	0.217%
22	7.710	915	922	928	rVB2	168967	205401	6.60%	1.011%
23	7.816	937	940	945	rVB4	31239	48307	1.55%	0.238%
24	7.869	945	949	951	rBV2	84294	85825	2.76%	0.422%
25	7.975	964	967	970	rBV3	46244	41982	1.35%	0.207%
26	8.069	977	983	987	rBV5	32181	43658	1.40%	0.215%
27	8.139	987	995	998	rBV	834697	778737	25.02%	3.833%
28	8.204	1004	1006	1011	rVB5	29427	43448	1.40%	0.214%
29	8.334	1024	1028	1033	rBV5	36049	51118	1.64%	0.252%
30	8.410	1039	1041	1047	rVB4	32441	57366	1.84%	0.282%
31	8.516	1053	1059	1064	rVB5	30425	46186	1.48%	0.227%
32	8.857	1113	1117	1123	rBV7	20248	44812	1.44%	0.221%
33	8.951	1127	1133	1136	rBV	86358	96428	3.10%	0.475%
34	9.216	1173	1178	1181	rBV	3462215	3112513	100.00%	15.320%
35	9.322	1192	1196	1200	rBV2	29740	37713	1.21%	0.186%
36	9.410	1209	1211	1219	rVB2	50478	55917	1.80%	0.275%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
Data File : BF128379.D
Acq On : 20 May 2022 22:35
Operator : CG\JU
Sample : N2943-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

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-BF052022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.557	1232	1236	1241	rVB6	24341	34153	1.10%	0.168%
38	9.610	1242	1245	1248	rVV	409271	299246	9.61%	1.473%
39	9.810	1274	1279	1284	rVB2	40458	50959	1.64%	0.251%
40	9.898	1290	1294	1297	rBV	952010	790123	25.39%	3.889%
41	10.216	1344	1348	1354	rBV8	17657	36181	1.16%	0.178%
42	10.692	1425	1429	1442	rBV	2062405	1916390	61.57%	9.433%
43	11.392	1544	1548	1551	rBV	831693	730013	23.45%	3.593%
44	11.910	1633	1636	1640	rBV2	71183	71594	2.30%	0.352%
45	12.980	1813	1818	1821	rBV	2623966	2377492	76.38%	11.702%
46	13.886	1966	1972	1979	rBV2	73574	122643	3.94%	0.604%
47	14.039	1994	1998	2002	rBV	552226	484095	15.55%	2.383%
48	14.139	2012	2015	2019	rVB	71325	68880	2.21%	0.339%
49	14.792	2123	2126	2131	rVB	39247	44166	1.42%	0.217%
50	15.133	2181	2184	2189	rVB	43432	47229	1.52%	0.232%
51	15.527	2245	2251	2259	rVB	422651	552467	17.75%	2.719%
52	15.957	2319	2324	2329	rVB2	34929	53247	1.71%	0.262%

Sum of corrected areas: 20316137

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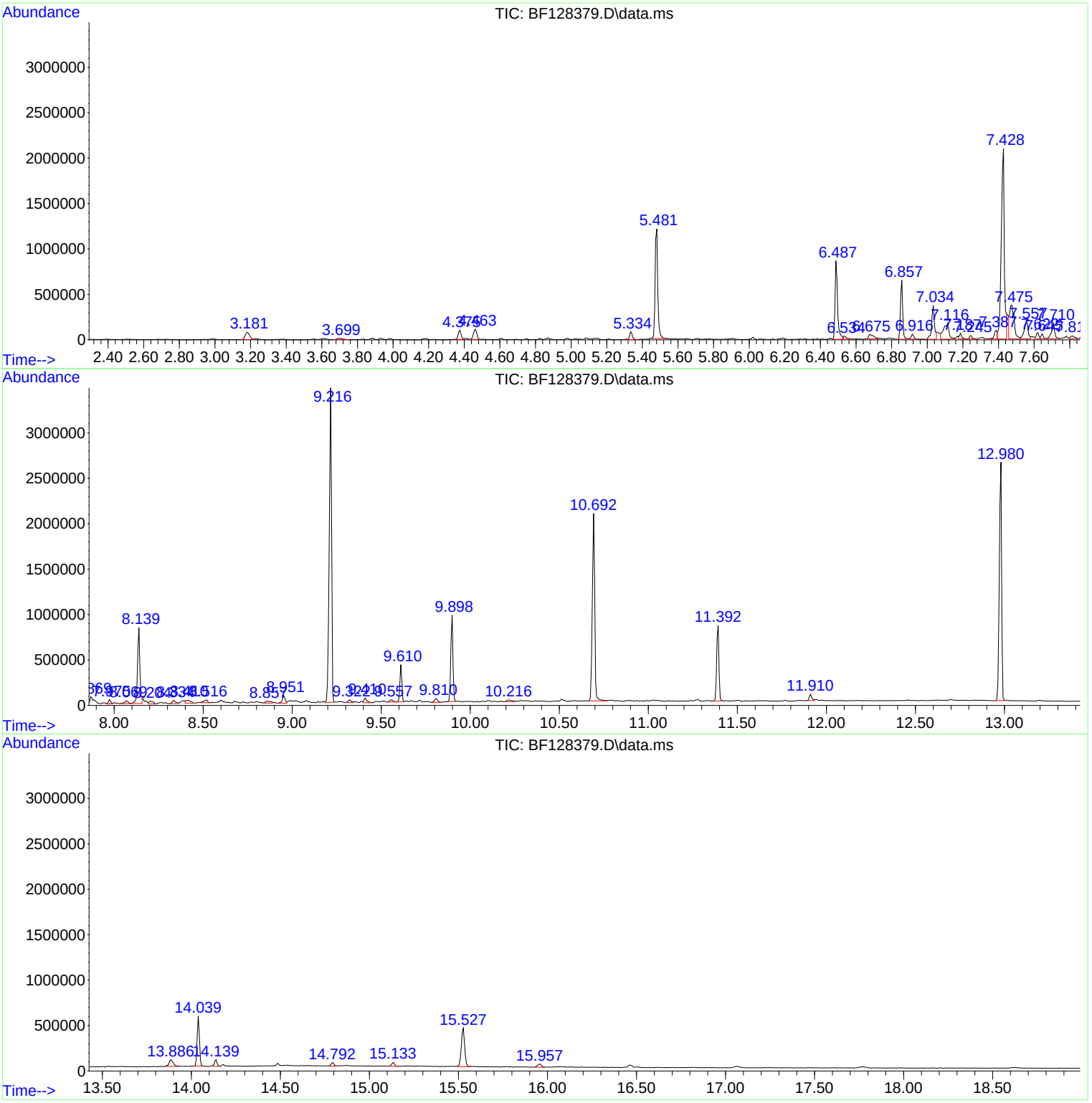
Instrument :
BNA_F
ClientSampleId :
MW-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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\BF052022\
Data File : BF128379.D
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Operator : CG\JU
Sample : N2943-15
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

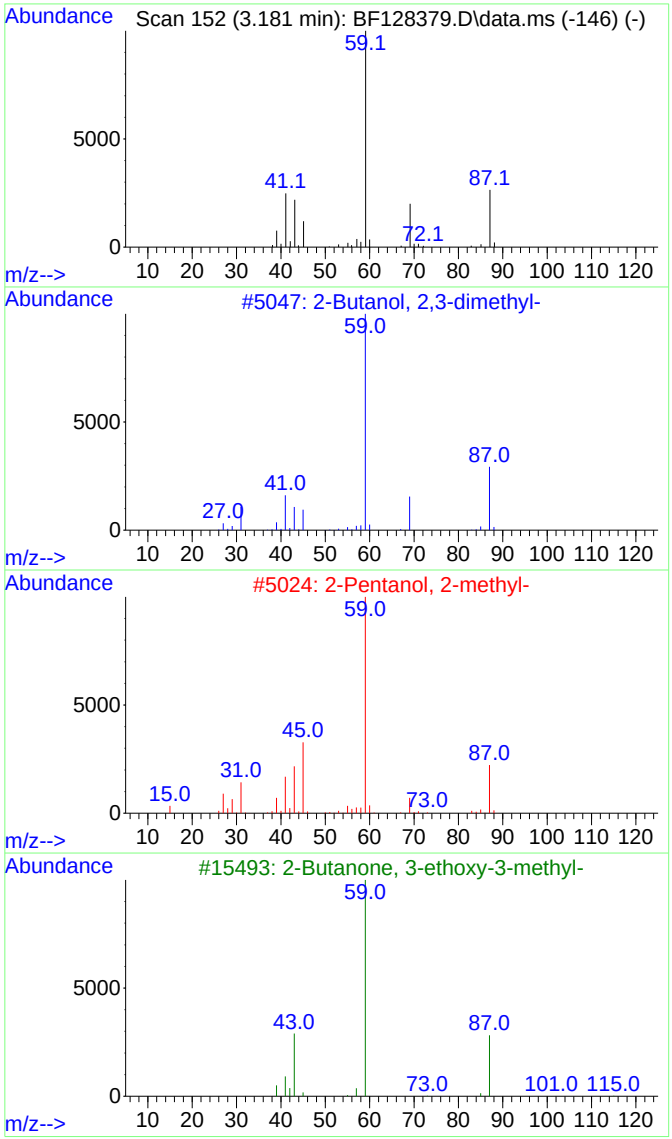
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

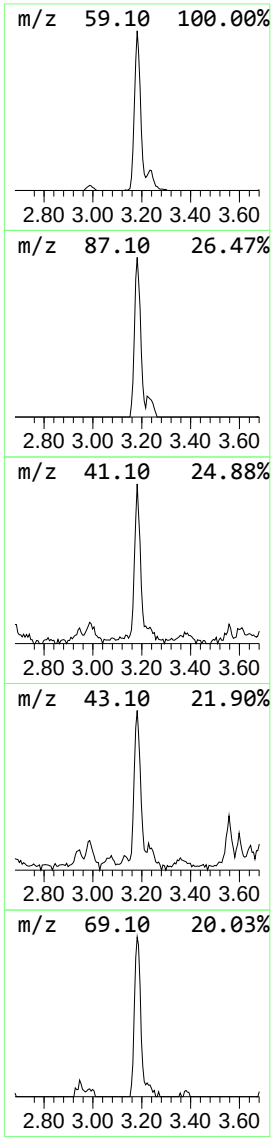
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.181	4.98 ng	140456	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	83
3	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	50
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
5	3-Heptanol	116	C7H16O	000589-82-2	40





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

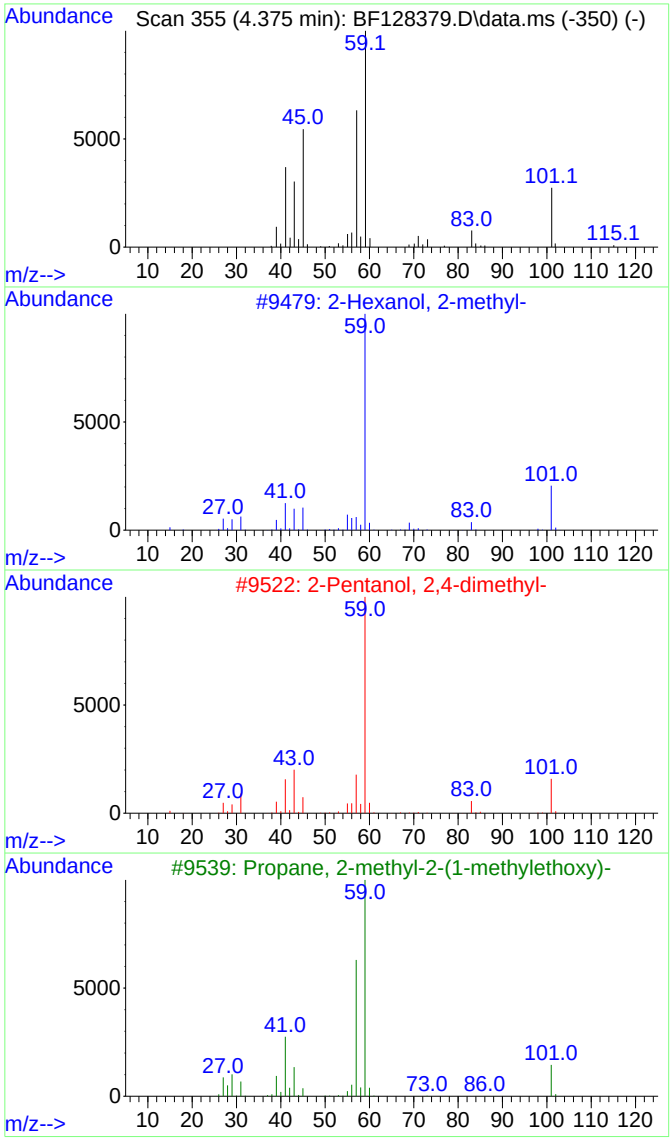
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

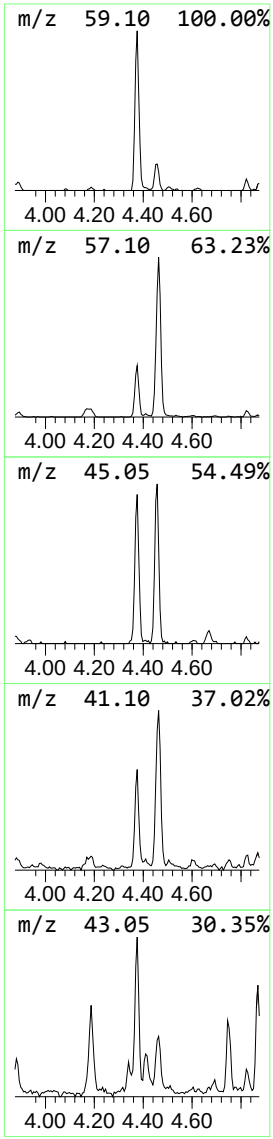
****

Peak Number 2 2-Hexanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.375	4.11 ng	116043	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	53
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
4	2-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	019780-63-3	47
5	3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	45





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Data File : BF128379.D
Acq On : 20 May 2022 22:35
Operator : CG\JU
Sample : N2943-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

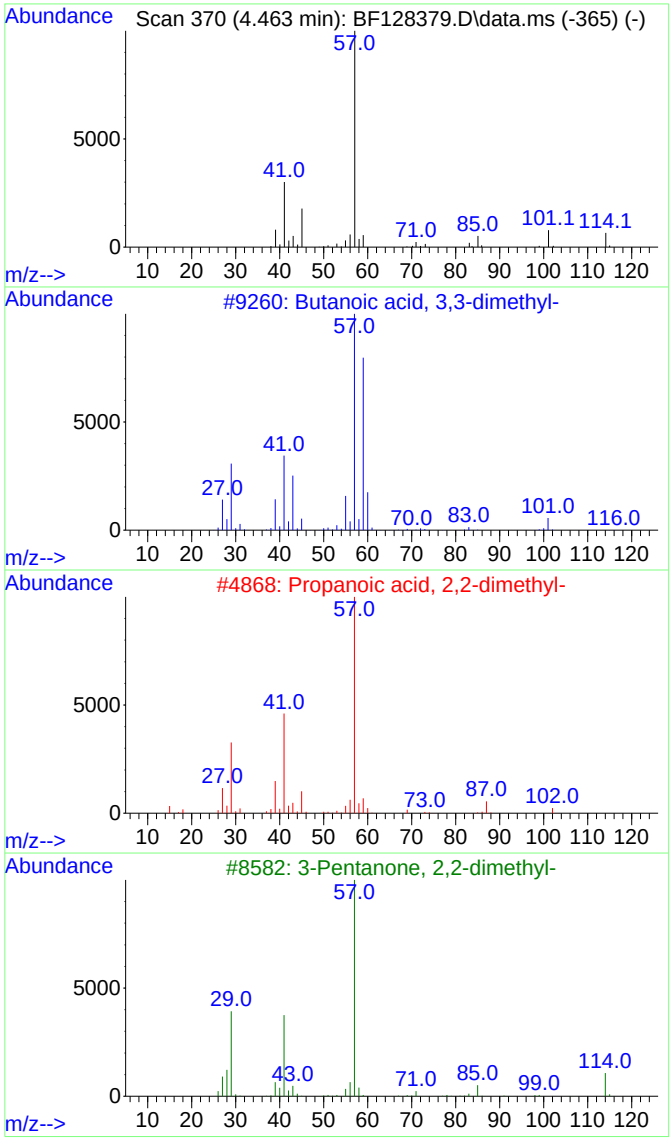
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

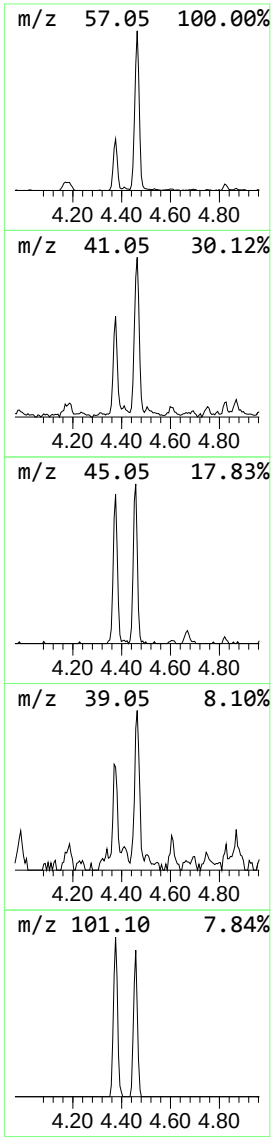
****

Peak Number 3 unknown4.463 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	5.32 ng	150145	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	38
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
3	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	38
4	Pivalic acid vinyl ester	128	C7H12O2	003377-92-2	37
5	3-Heptanone	114	C7H14O	000106-35-4	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
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Operator : CG\JU
Sample : N2943-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

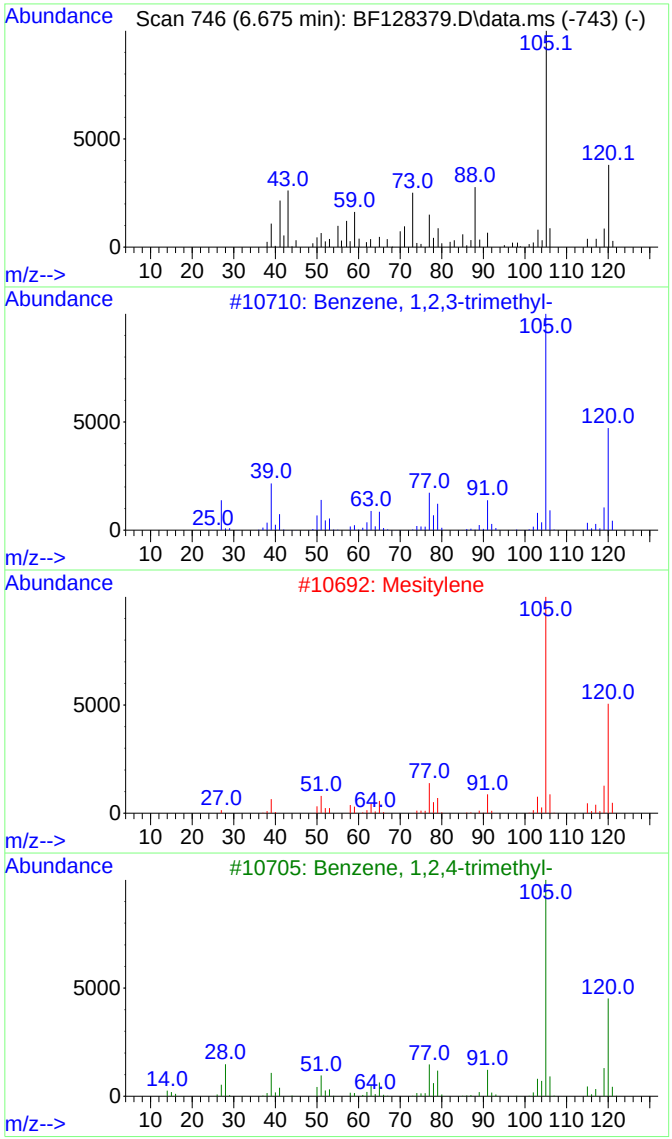
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

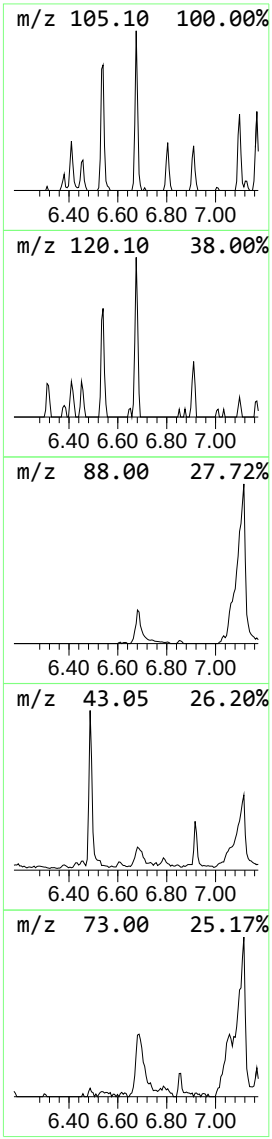
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.675	3.61 ng	101806	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	50
2	Mesitylene	120	C9H12	000108-67-8	50
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	49
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	49
5	Trimethylsilyl methyl sulfide	120	C4H12SSi	003908-55-2	47





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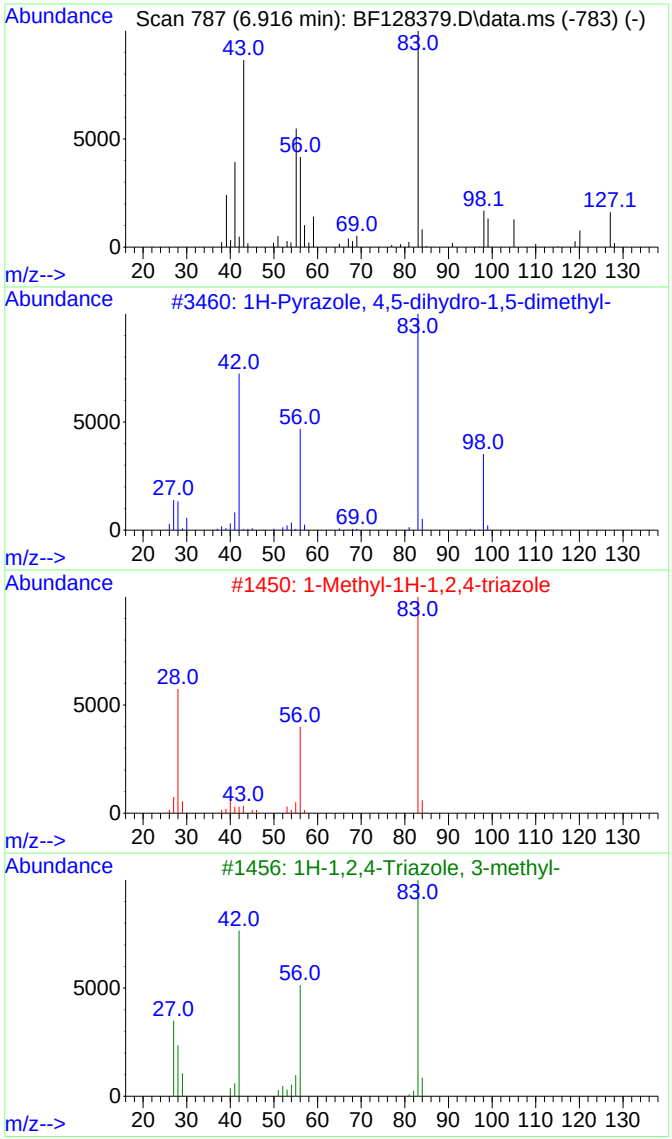
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

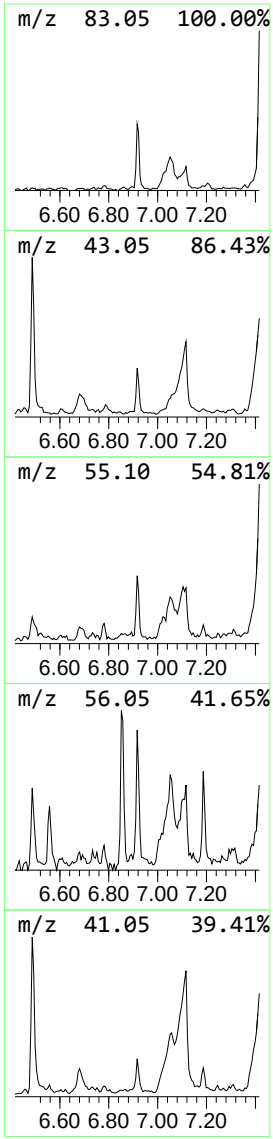
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Pyrazole, 4,5-dihydro-1,... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.916	2.05 ng	57829	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	53
2	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	50
3	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	50
4	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	47
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	46





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

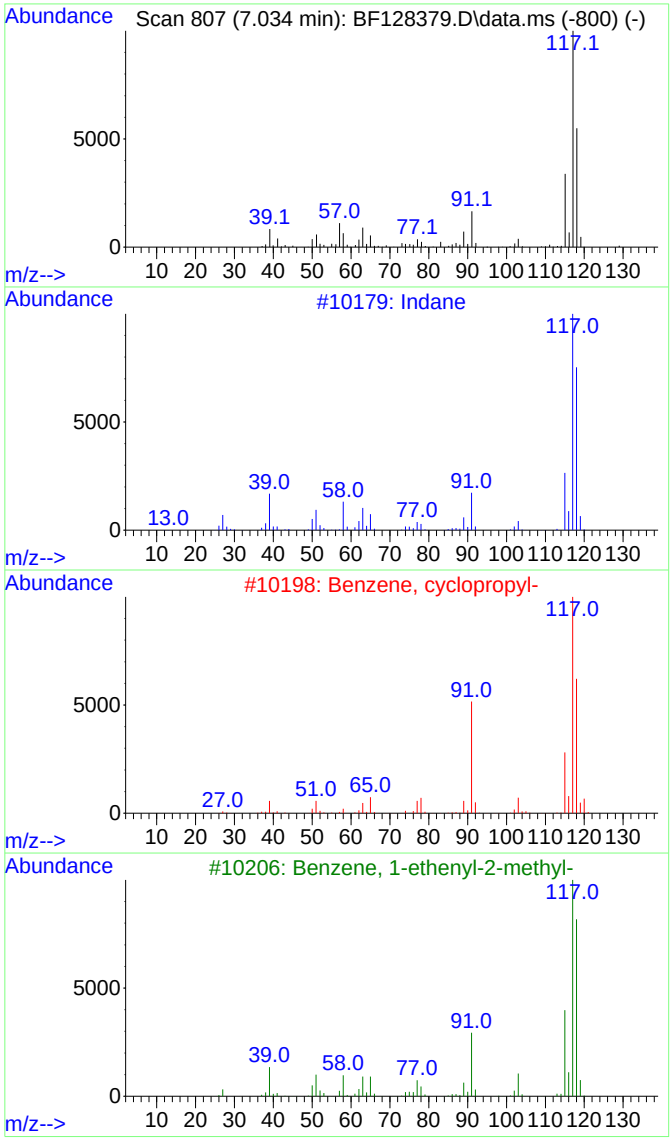
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

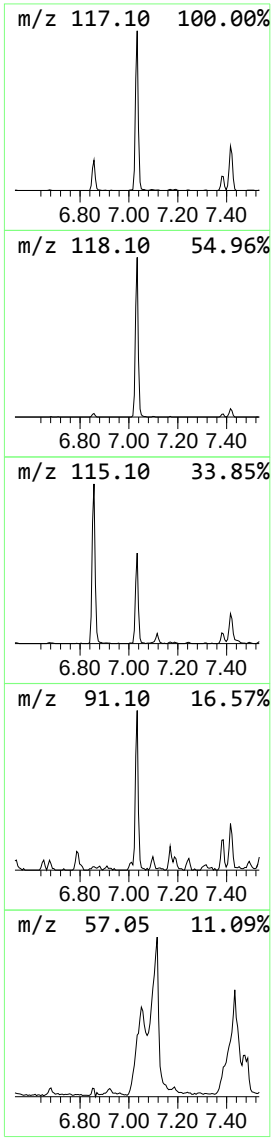
****

Peak Number 7 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	14.64 ng	413078	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	53
5	Deltacyclene	118	C9H10	007785-10-6	50





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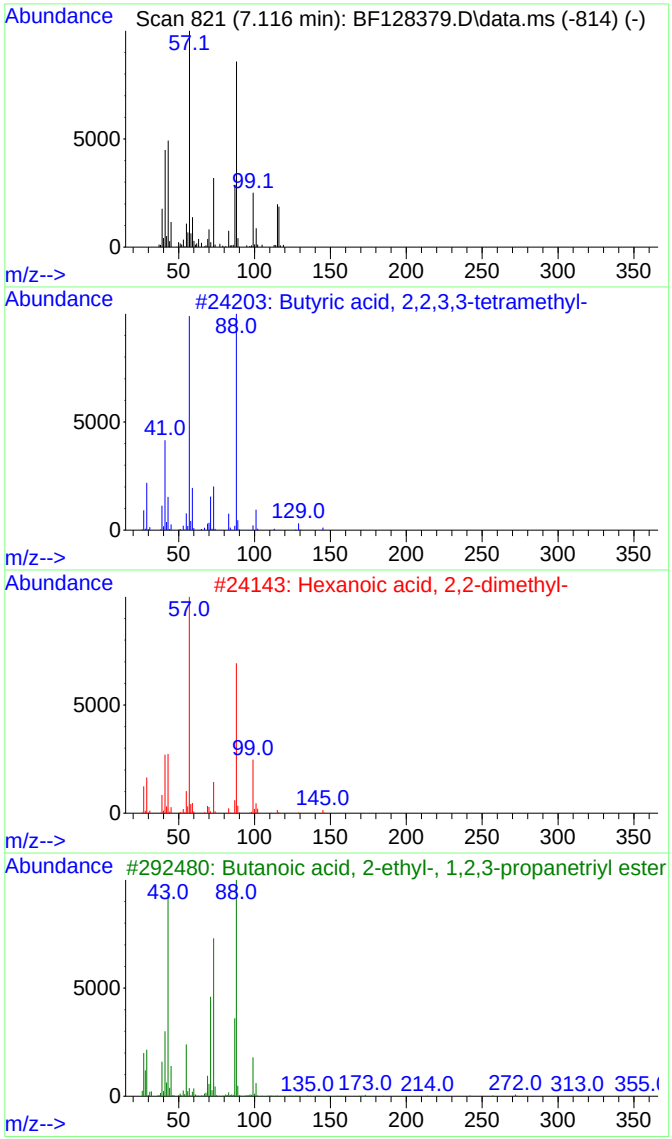
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

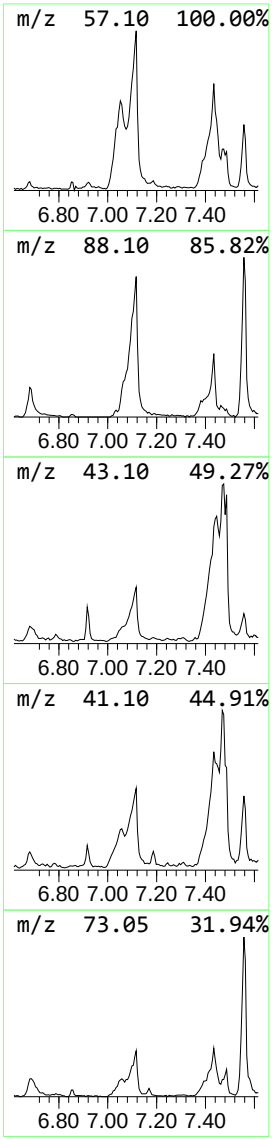
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butyric acid, 2,2,3,3-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.116	13.33 ng	376096	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	50
2	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	42
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
4	Methyl (R)-(-)-3-hydroxy-2-methy...	118	C5H10O3	072657-23-9	37
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	37





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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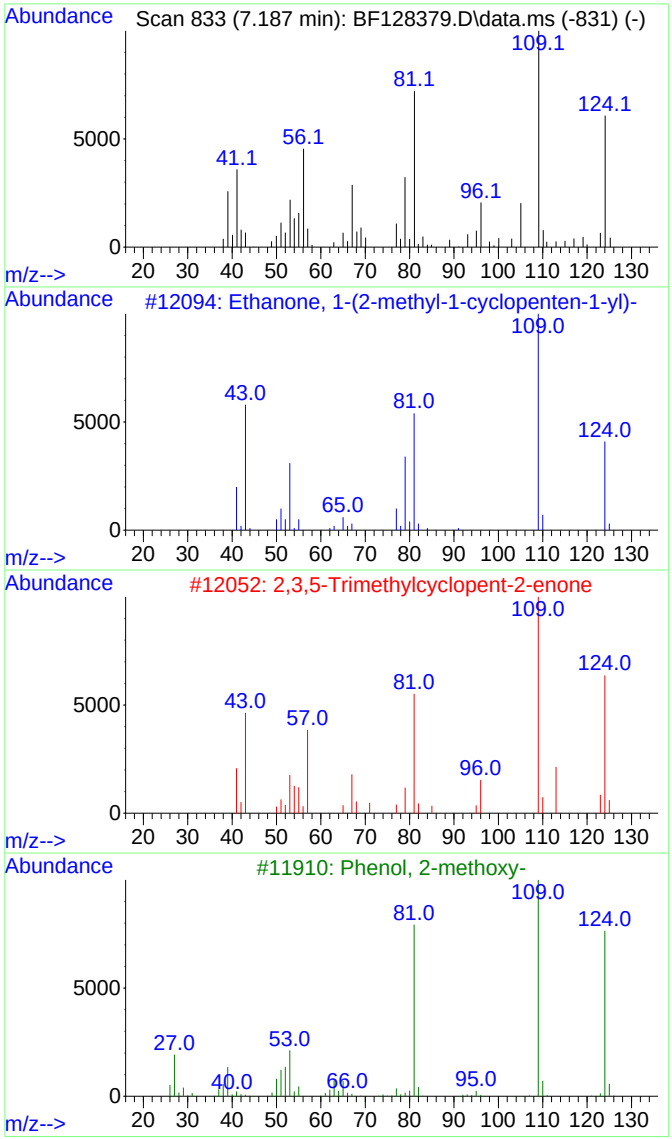
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

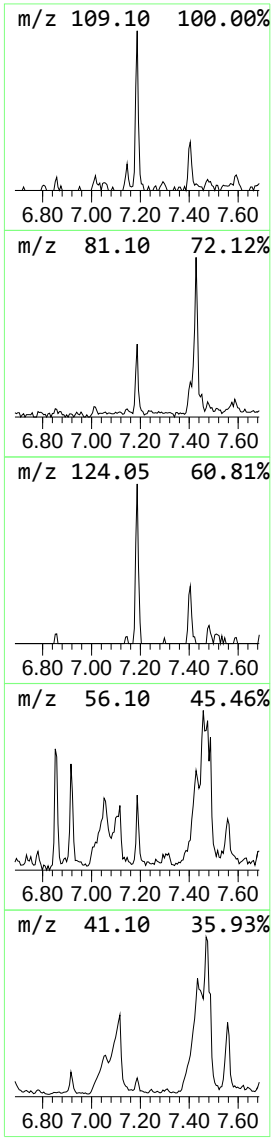
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Ethanone, 1-(2-methyl-1-cyc... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.187	2.07 ng	58281	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2-methyl-1-cyclopen...	124	C8H12O	003168-90-9	64
2	2,3,5-Trimethylcyclopent-2-enone	124	C8H12O	1000427-08-7	52
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	50
4	Mequinol	124	C7H8O2	000150-76-5	49
5	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	46





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Data File : BF128379.D
Acq On : 20 May 2022 22:35
Operator : CG\JU
Sample : N2943-15
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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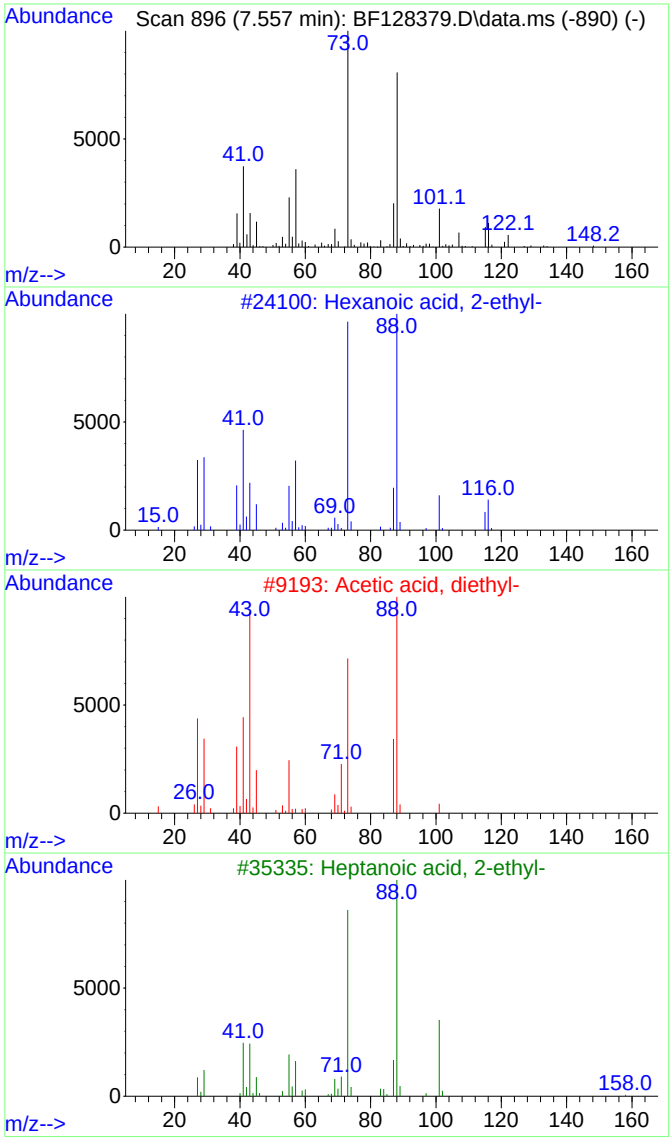
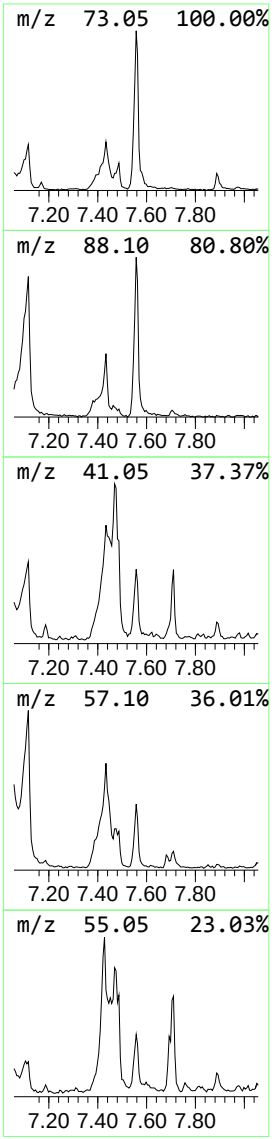
Peak Number 10 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.557	7.26 ng	282711	Naphthalene-d8	8.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	53
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	40
4	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	40
5	1,4-Dioxane	88	C4H8O2	000123-91-1	38





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Sample : N2943-15
Misc :
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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

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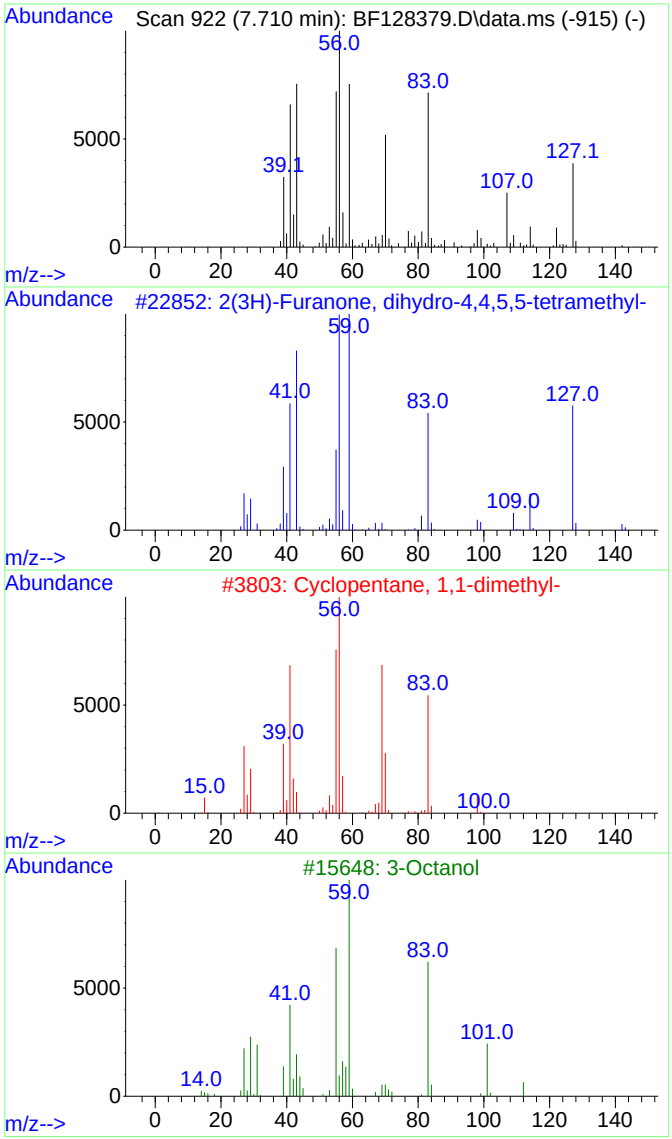
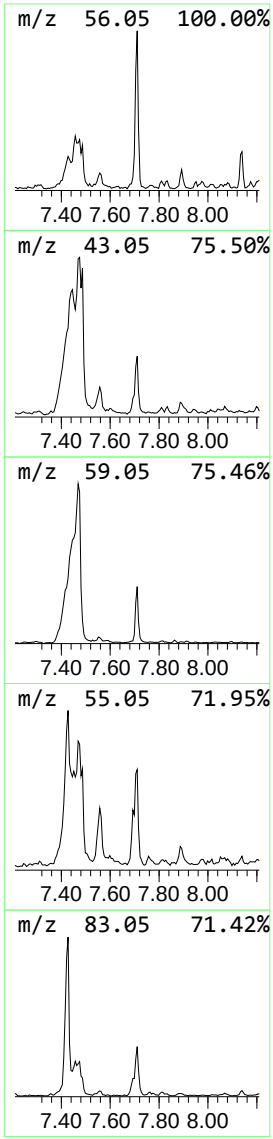
Peak Number 11 unknown7.710 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.710	5.28 ng	205401	Naphthalene-d8	8.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	43
2	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	42
3	3-Octanol	130	C8H18O	000589-98-0	22
4	1-Heptene	98	C7H14	000592-76-7	22
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	14





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Operator : CG\JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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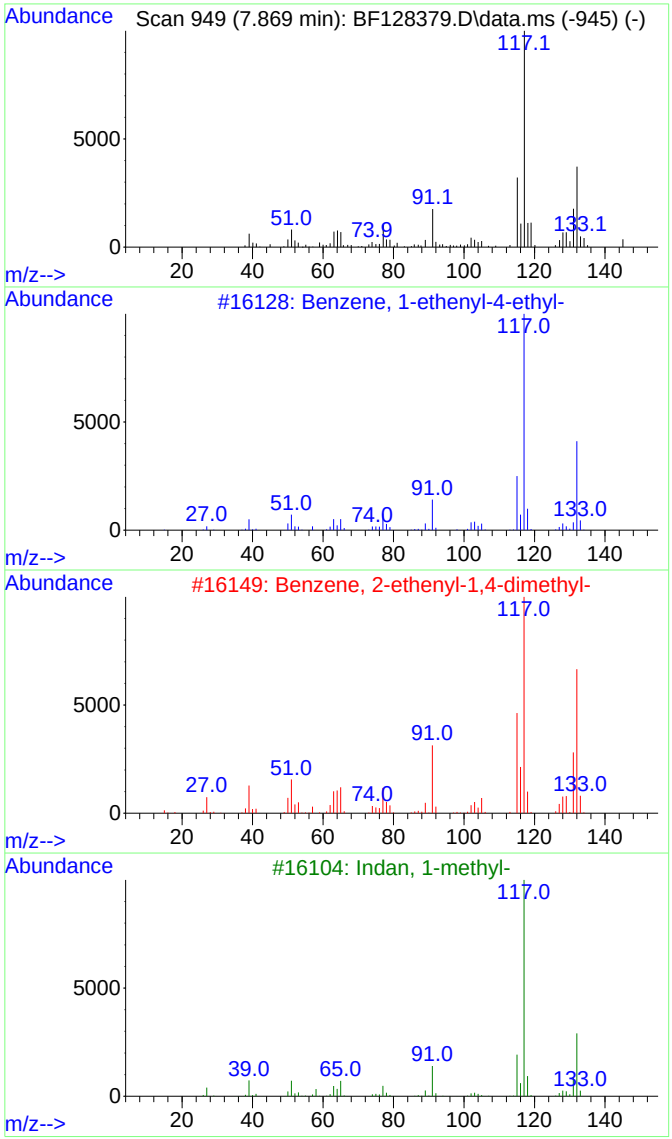
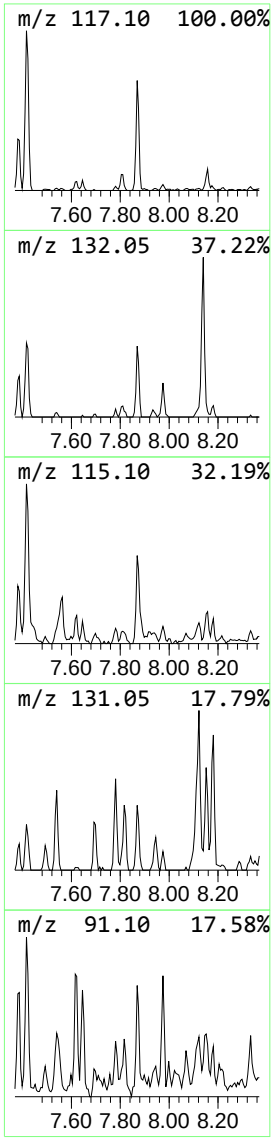
Peak Number 12 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.869	2.20 ng	85825	Naphthalene-d8	8.139

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	87





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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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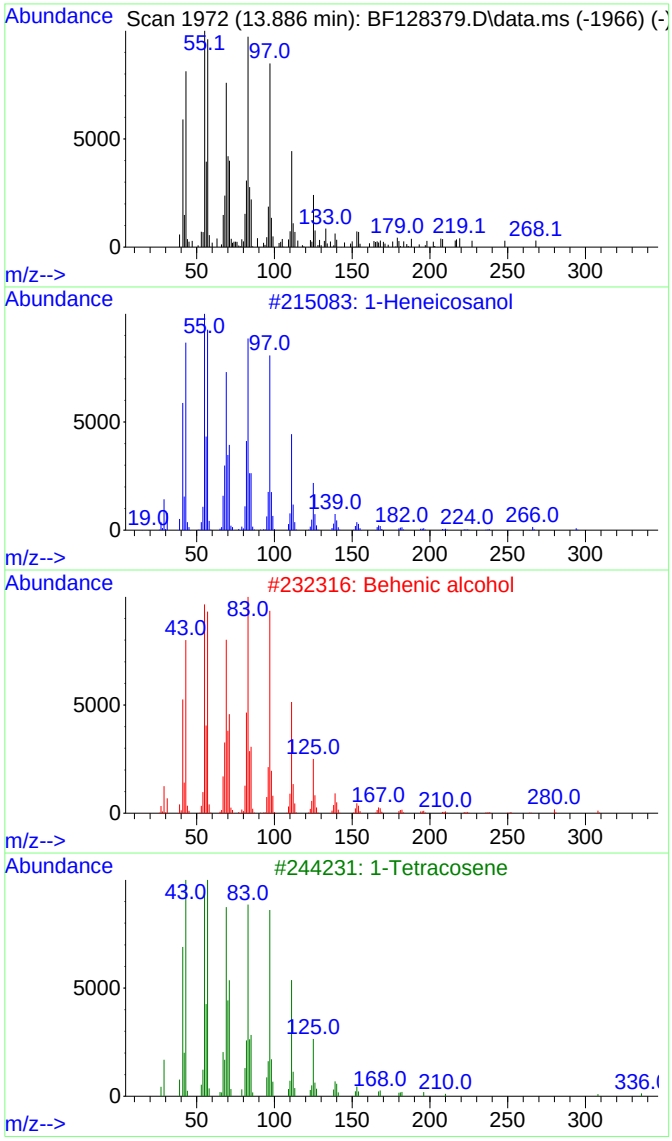
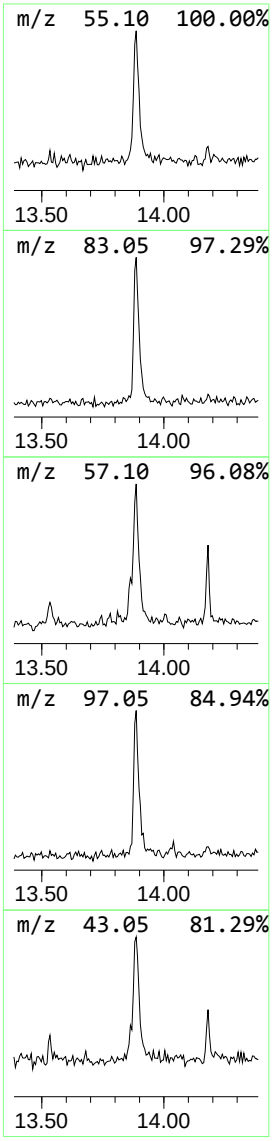
Peak Number 14 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.07 ng	122643	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Tetracosene	336	C24H48	010192-32-2	90
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.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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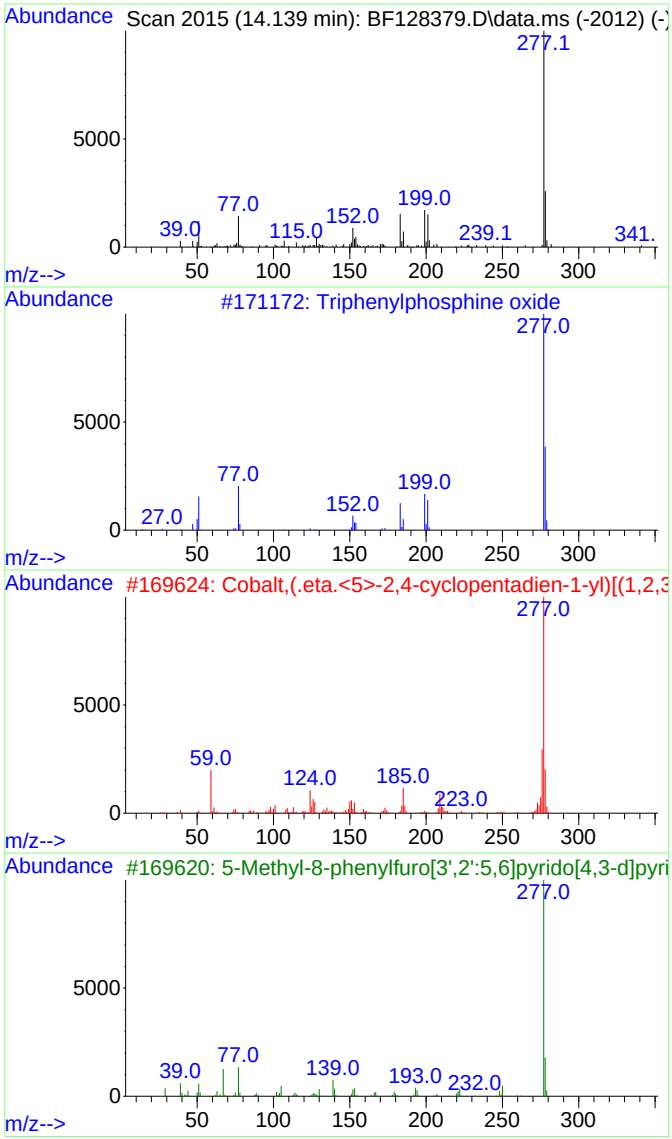
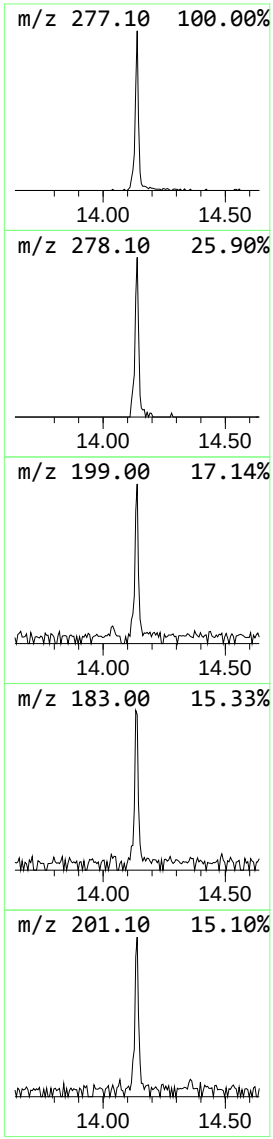
Peak Number 15 Triphenylphosphine oxide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.85 ng	68880	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	59
3	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	53
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	53
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Butanol, 2,3-...	3.181	5.0	ng	140456	1	6.857	564453	20.0
2-Hexanol, 2-me...	4.375	4.1	ng	116043	1	6.857	564453	20.0
unknown4.463	4.463	5.3	ng	150145	1	6.857	564453	20.0
Benzene, 1,2,3-...	6.675	3.6	ng	101806	1	6.857	564453	20.0
1H-Pyrazole, 4,...	6.916	2.0	ng	57829	1	6.857	564453	20.0
Indane	7.034	14.6	ng	413078	1	6.857	564453	20.0
Butyric acid, 2...	7.116	13.3	ng	376096	1	6.857	564453	20.0
Ethanone, 1-(2-...	7.187	2.1	ng	58281	1	6.857	564453	20.0
Hexanoic acid, ...	7.557	7.3	ng	282711	2	8.139	778737	20.0
unknown7.710	7.710	5.3	ng	205401	2	8.139	778737	20.0
Benzene, 1-ethe...	7.869	2.2	ng	85825	2	8.139	778737	20.0
1-Heneicosanol	13.886	5.1	ng	122643	5	14.039	484095	20.0
Triphenylphosph...	14.139	2.9	ng	68880	5	14.039	484095	20.0