LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
Data File : BF128384.D
Acq On : 21 May 2022 01:03
Operator : CG\JU
Sample : N2943-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

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: BF128384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.175	145	151	157	rBV	98114	170017	5.81%	0.936%
2	4.369	350	354	358	rBV	99007	118741	4.06%	0.654%
3	4.457	364	369	375	rVB2	103308	140283	4.79%	0.772%
4	4.869	434	439	446	rVB2	22115	33073	1.13%	0.182%
5	5.334	515	518	526	rVB	109587	110692	3.78%	0.609%
6	5.481	539	543	553	rVB	1480299	1343279	45.89%	7.396%
7	6.022	630	635	639	rBV	69009	60977	2.08%	0.336%
8	6.310	682	684	689	rVB	36918	34695	1.19%	0.191%
9	6.493	711	715	731	rBV	1032604	1002186	34.23%	5.518%
10	6.681	740	747	753	rBV4	34767	66548	2.27%	0.366%
11	6.857	773	777	784	rBV	666277	540042	18.45%	2.974%
12	6.922	784	788	794	rVB	57689	60962	2.08%	0.336%
13	7.034	800	807	811	rBV	331051	334132	11.41%	1.840%
14	7.098	811	818	824	rVV3	138536	253546	8.66%	1.396%
15	7.187	828	833	840	rVB3	44521	57240	1.96%	0.315%
16	7.428	858	874	877	rBV	2041072	2366066	80.82%	13.028%
17	7.457	877	879	884	rVB2	253497	276644	9.45%	1.523%
18	7.545	890	894	900	rVB2	34354	50765	1.73%	0.280%
19	7.710	916	922	927	rBV	161554	164543	5.62%	0.906%
20	7.810	936	939	946	rVB5	23156	37679	1.29%	0.207%
21	7.869	946	949	956	rBV4	35979	60557	2.07%	0.333%
22	7.975	964	967	970	rBV2	36821	32785	1.12%	0.181%
23	8.140	991	995	998	rBV	786091	655713	22.40%	3.610%
24	8.204	1004	1006	1011	rVB4	29198	33601	1.15%	0.185%
25	8.334	1024	1028	1032	rBV4	19451	33652	1.15%	0.185%
26	8.857	1113	1117	1128	rVB9	24085	59259	2.02%	0.326%
27	8.951	1128	1133	1137	rBV3	71508	84558	2.89%	0.466%
28	9.216	1173	1178	1181	rBV	3244528	2927449	100.00%	16.119%
29	9.410	1208	1211	1219	rVB2	47363	58434	2.00%	0.322%
30	9.810	1275	1279	1283	rVB2	24858	35030	1.20%	0.193%
31	9.898	1290	1294	1297	rBV	806006	681477	23.28%	3.752%
32	10.692	1425	1429	1437	rBV	1959815	1800616	61.51%	9.914%
33	11.392	1544	1548	1551	rBV	754722	652678	22.30%	3.594%
34	11.769	1609	1612	1618	rVB	91253	74995	2.56%	0.413%
35	11.910	1633	1636	1646	rBV3	34445	43135	1.47%	0.238%
36	12.475	1729	1732	1737	rVB	122495	117322	4.01%	0.646%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
Data File : BF128384.D
Acq On : 21 May 2022 01:03
Operator : CG\JU
Sample : N2943-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

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	12.980	1813	1818	1821	rBV	2576892	2391305	81.69%	13.167%
38	14.039	1994	1998	2002	rBV	539879	462333	15.79%	2.546%
39	14.139	2012	2015	2019	rVB	70445	62402	2.13%	0.344%
40	15.133	2181	2184	2188	rVB2	33294	34092	1.16%	0.188%
41	15.527	2245	2251	2258	rVB	404318	541929	18.51%	2.984%
42	15.957	2320	2324	2330	rVB2	33539	50448	1.72%	0.278%
43	16.468	2407	2411	2416	rVB2	27908	45807	1.56%	0.252%

Sum of corrected areas: 18161687

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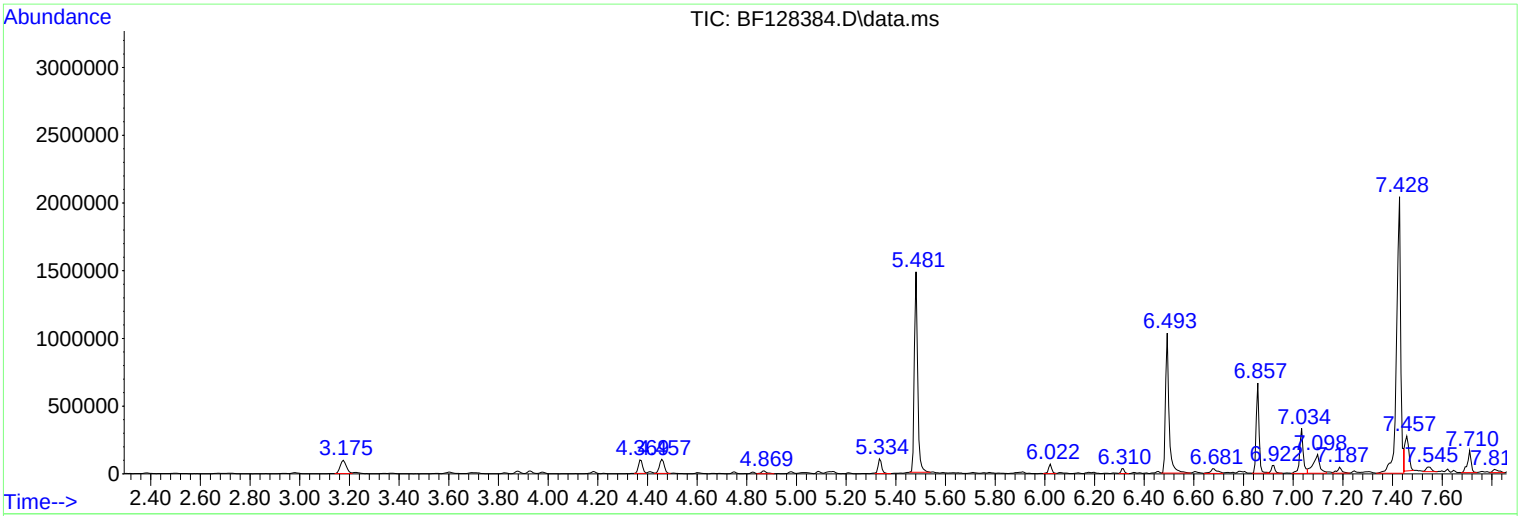
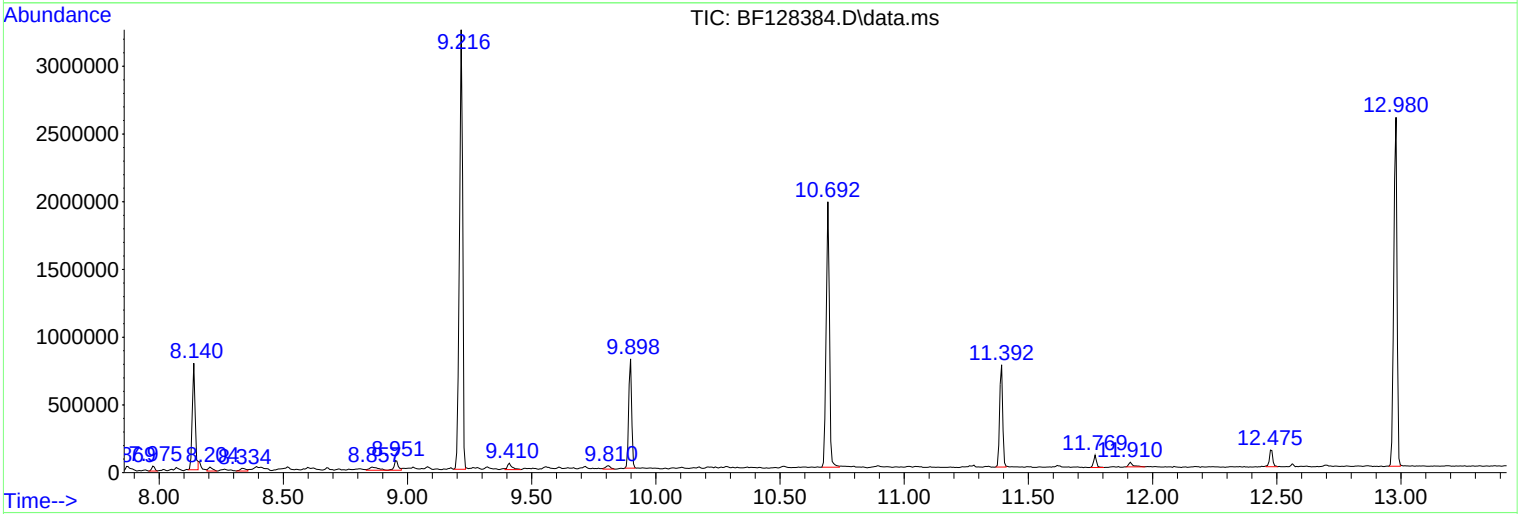
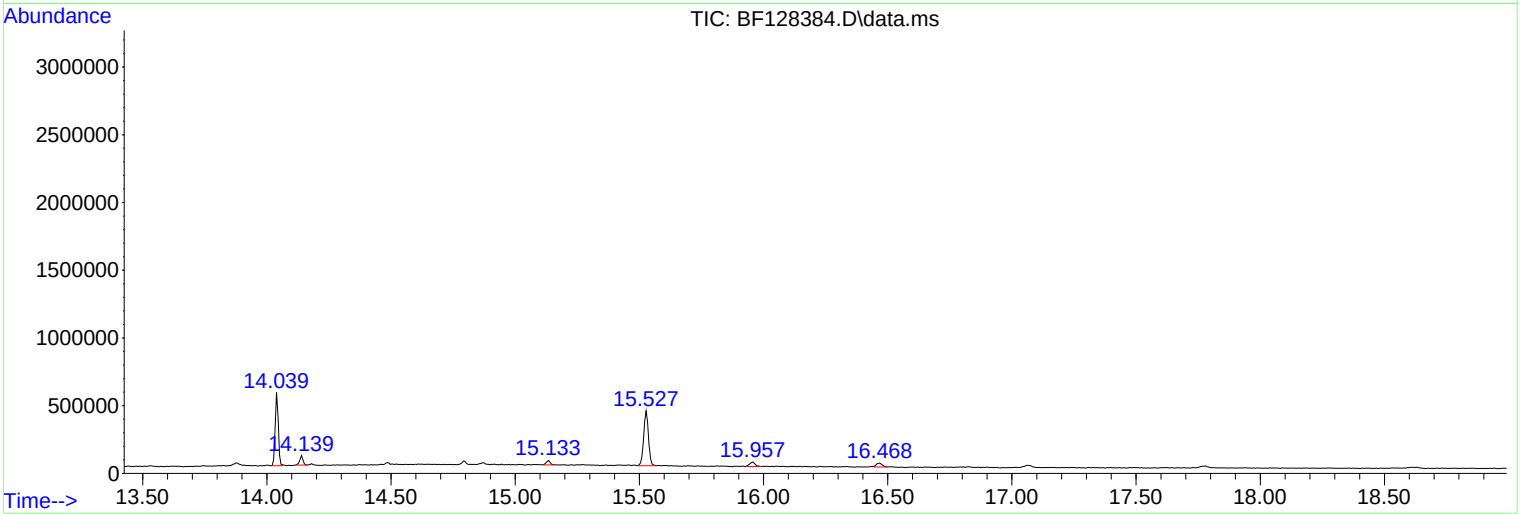
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF128384.D
Acq On : 21 May 2022 01:03
Operator : CG\JU
Sample : N2943-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

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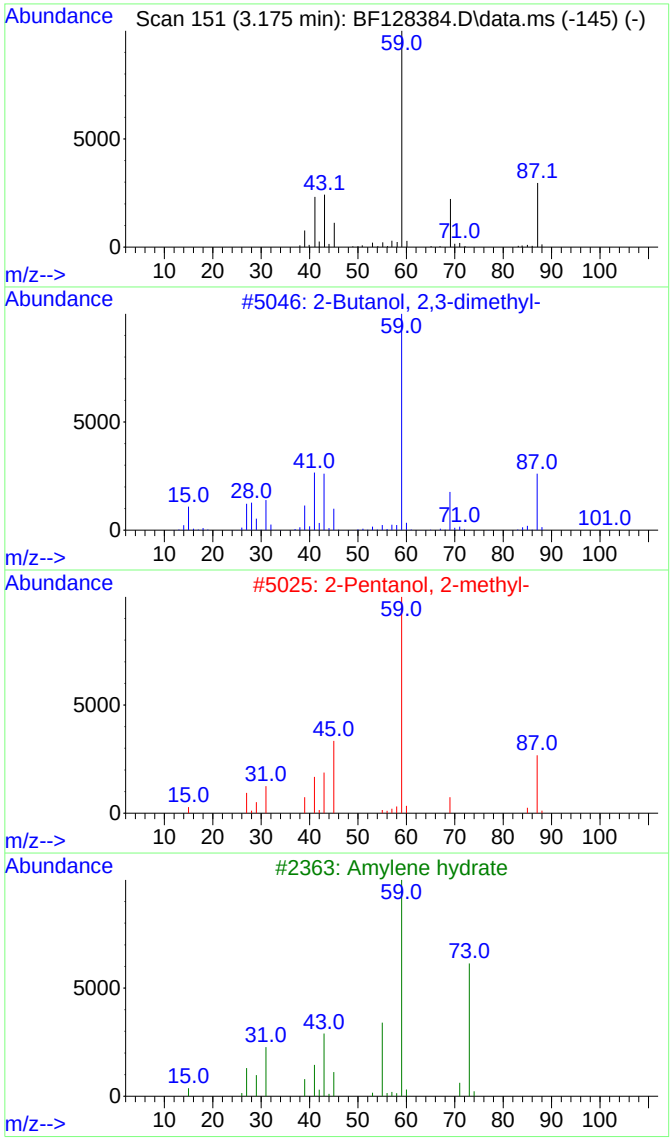
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

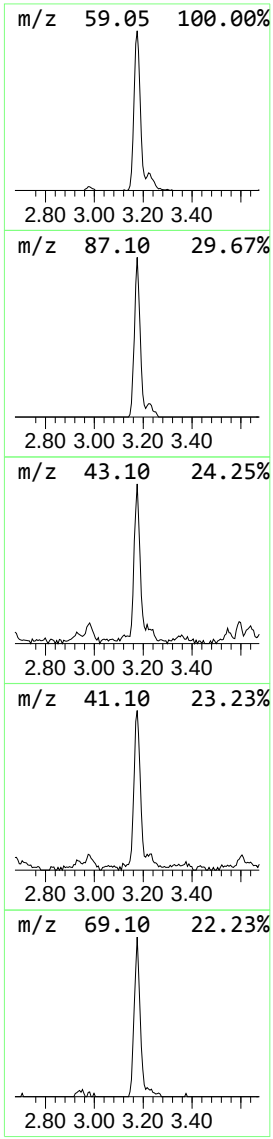
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	6.30 ng	170017	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	72
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3	Amylene hydrate	88	C5H12O	000075-85-4	42
4	3-Heptanol	116	C7H16O	000589-82-2	40
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39





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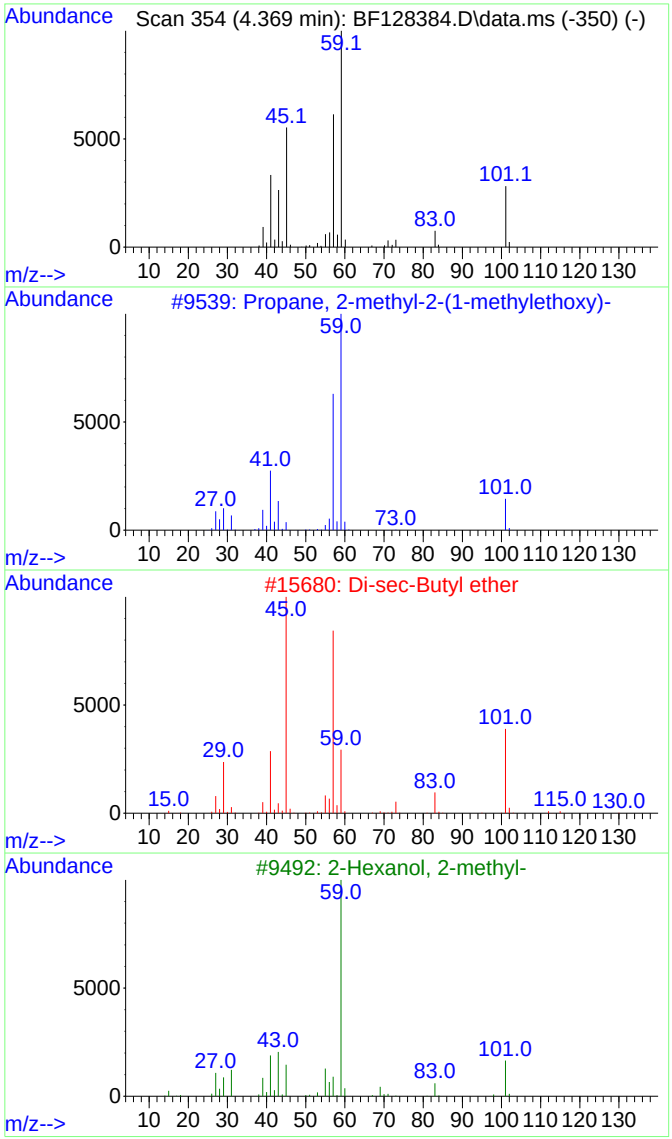
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

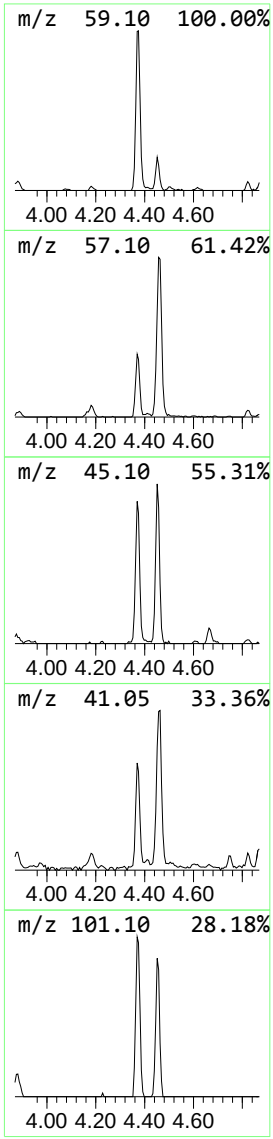
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.369	4.40 ng	118741	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	43
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
5	Ethyl ether	74	C4H10O	000060-29-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
Data File : BF128384.D
Acq On : 21 May 2022 01:03
Operator : CG\JU
Sample : N2943-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

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

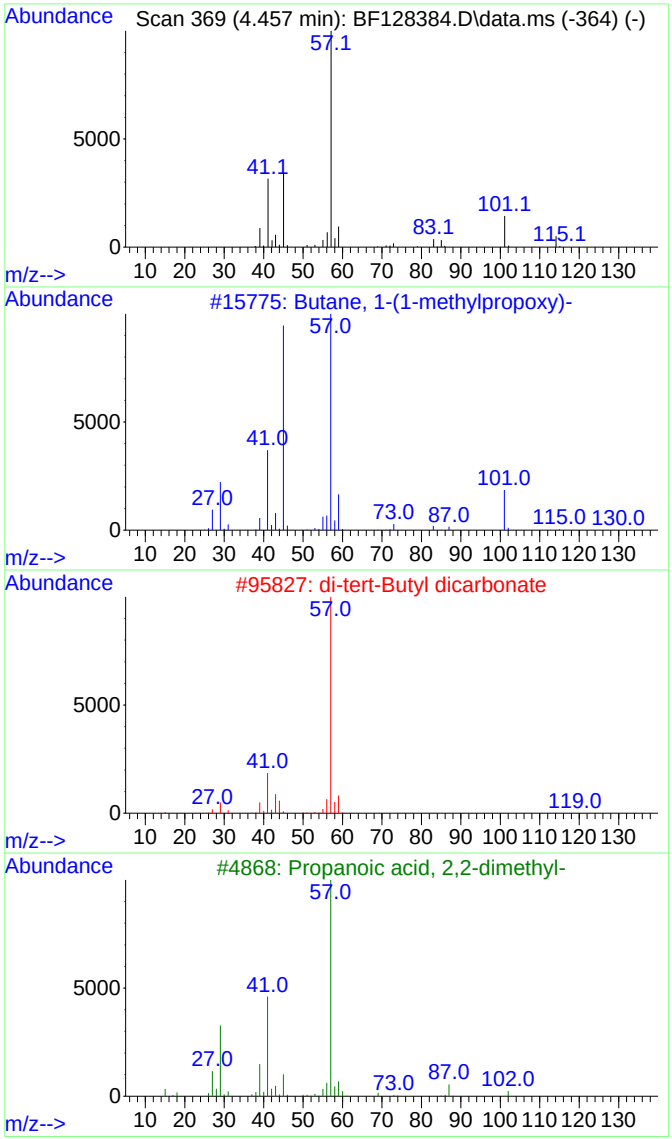
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

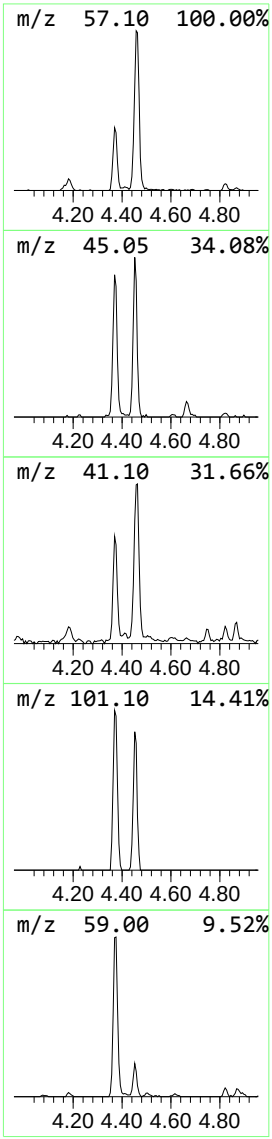
****

Peak Number 3 unknown4.457 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	5.20 ng	140283	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	45
2	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	38
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	32
4	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	25
5	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	25





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Misc :
ALS Vial : 19 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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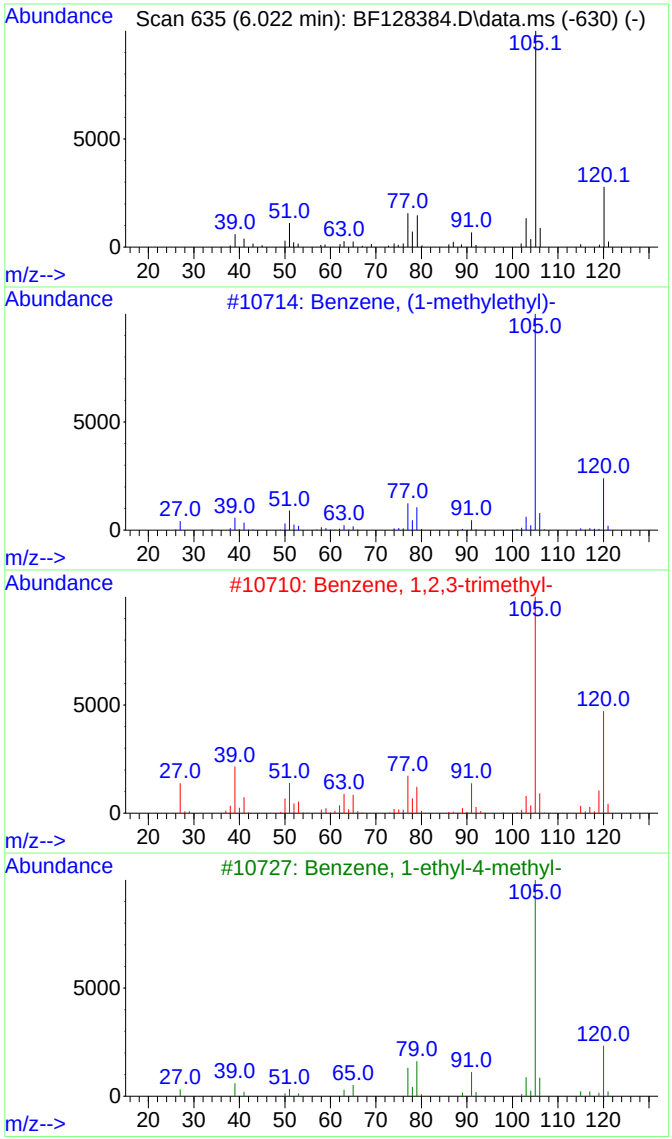
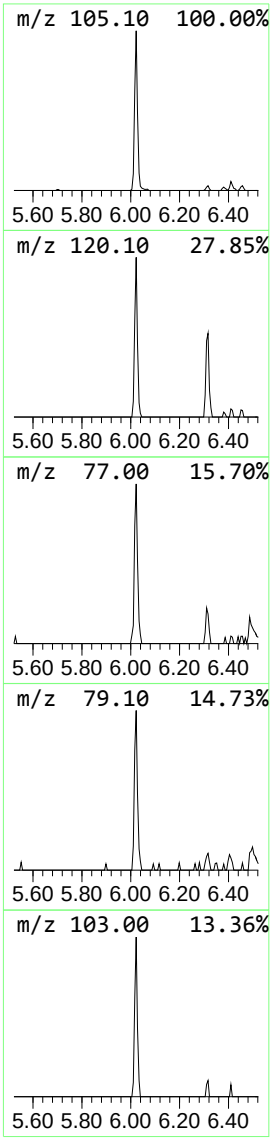
Peak Number 5 Benzene, (1-methylethyl)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.022	2.26 ng	60977	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	94
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	80
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	74
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	72





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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
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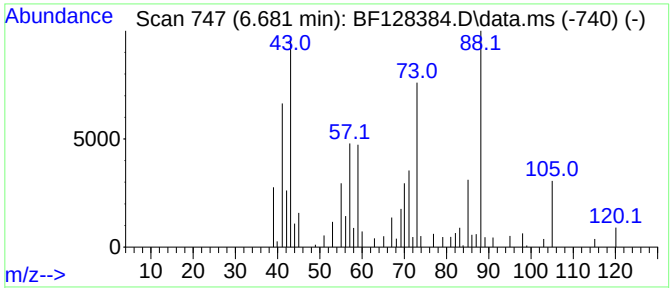
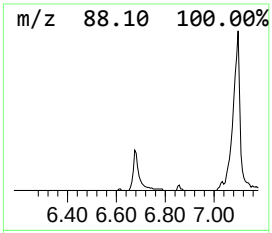
****

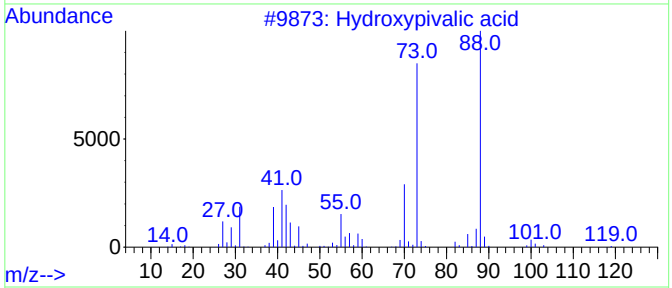
Peak Number 6 unknown6.681 Concentration Rank 11

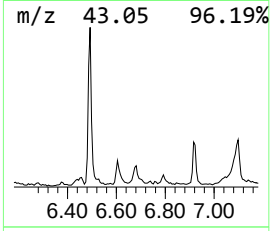
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	2.46 ng	66548	1,4-Dichlorobenzene-d4	6.857

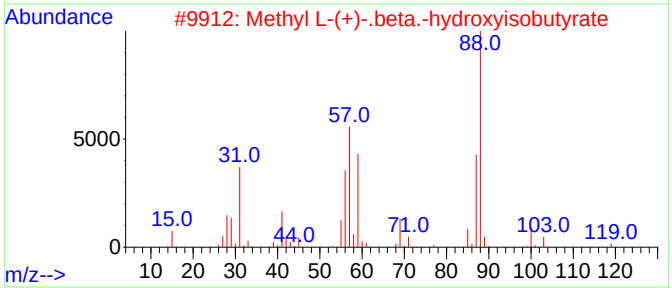
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydroxypivalic acid	118	C5H10O3	004835-90-9	38
2	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	38
3	Methyl (R)-(-)-3-hydroxy-2-methy...	118	C5H10O3	072657-23-9	38
4	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	38
5	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	35

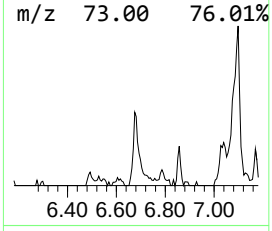


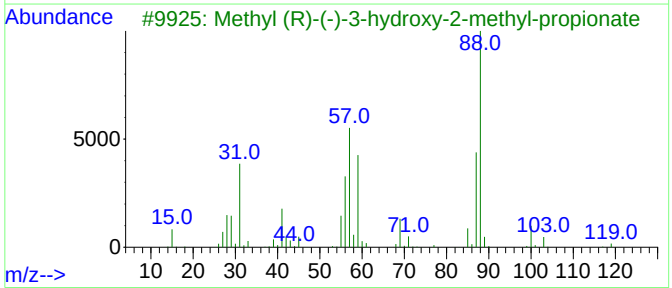


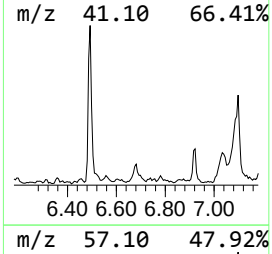


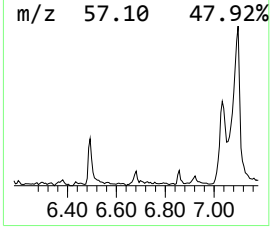












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

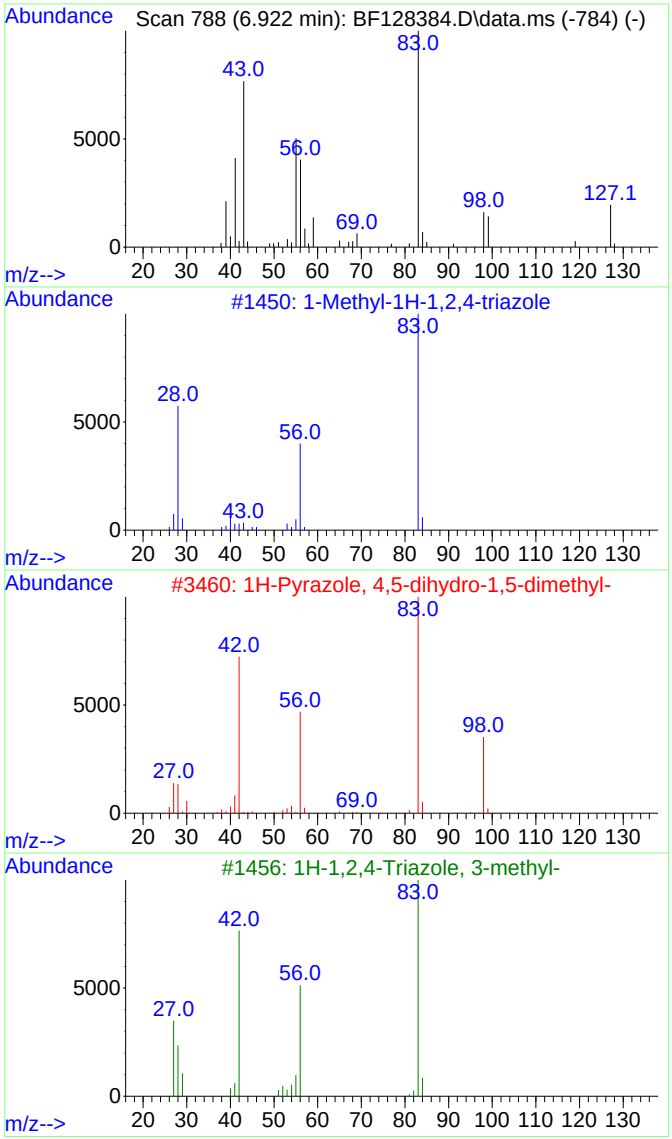
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

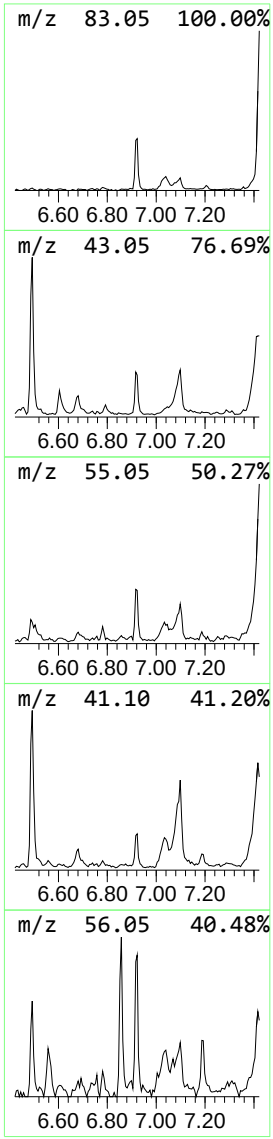
****

Peak Number 7 1-Methyl-1H-1,2,4-triazole Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.922	2.26 ng	60962	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	50
2	1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	50
3	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	47
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	43
5	Acetaldehyde 2E-hexenyl 3Z-hexen...	226	C14H26O2	1000431-45-5	43





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

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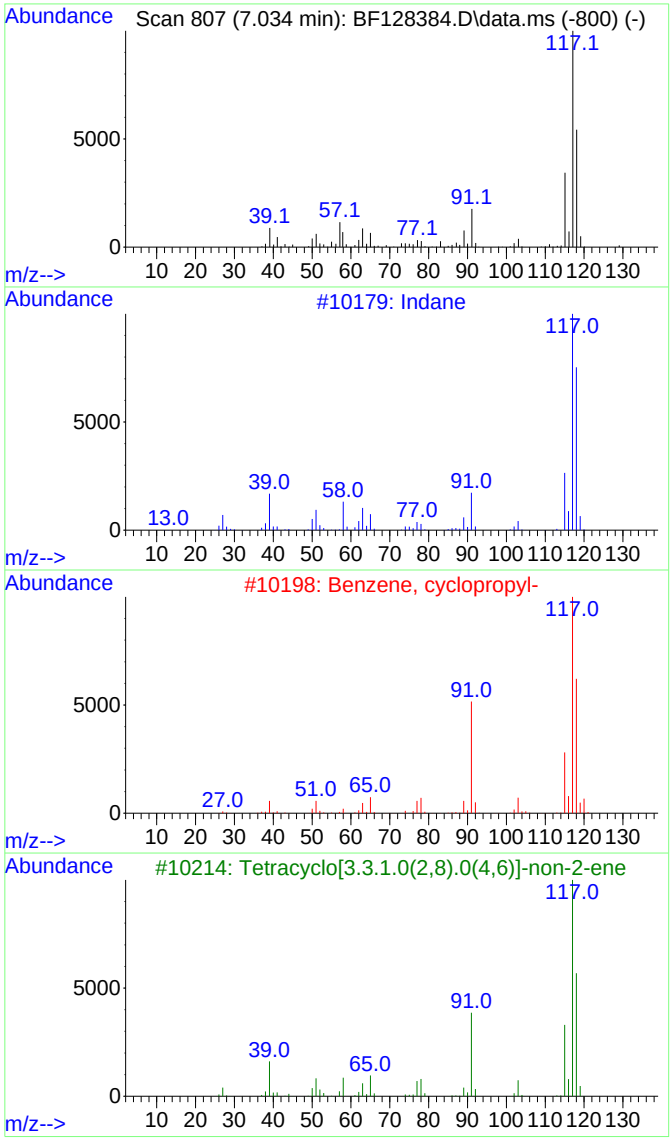
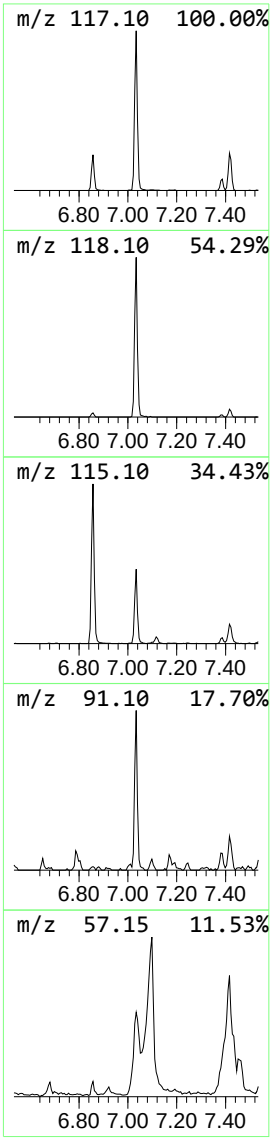
Peak Number 8 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	12.37 ng	334132	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	74
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	59
5	Deltacyclene	118	C9H10	007785-10-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052022\
Data File : BF128384.D
Acq On : 21 May 2022 01:03
Operator : CG\JU
Sample : N2943-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-35

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

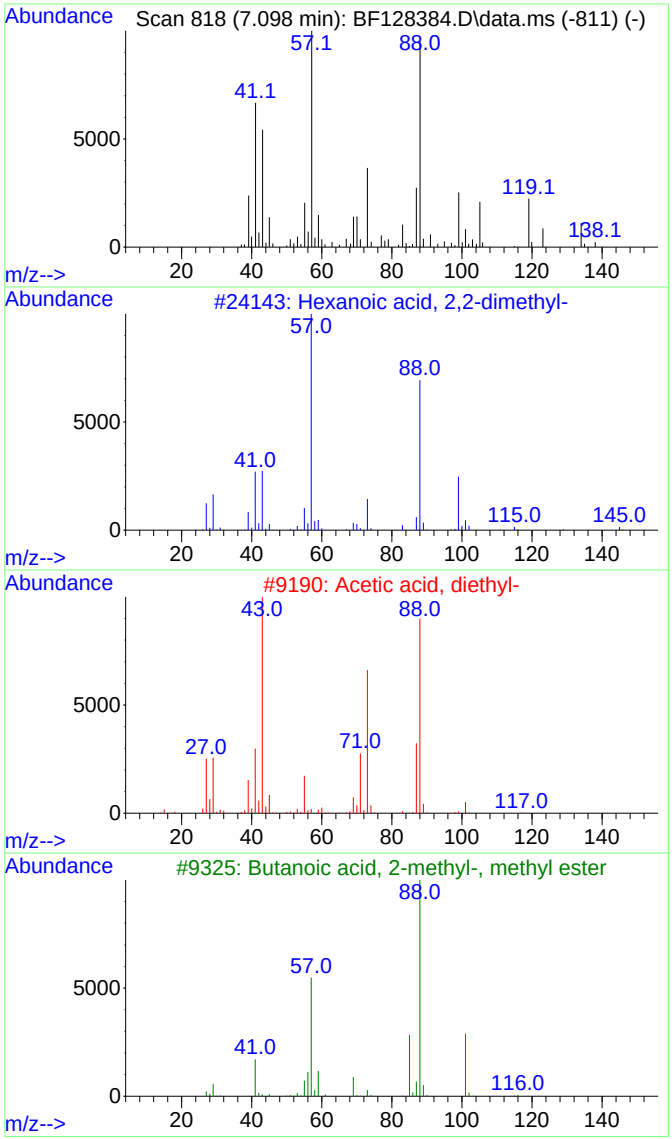
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

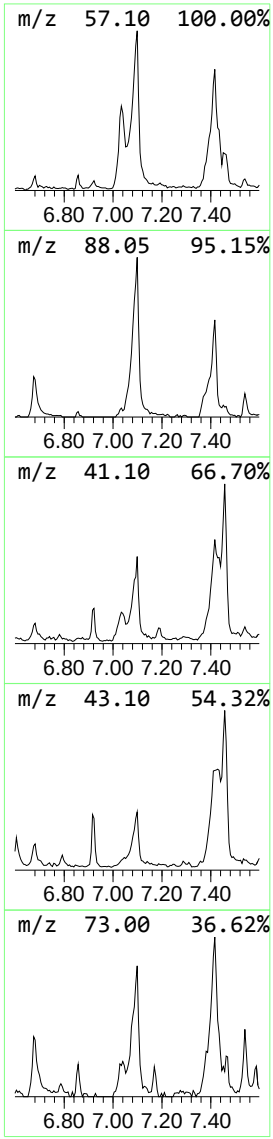
****

Peak Number 9 unknown7.098 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.098	9.39 ng	253546	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	47
2	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	38
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	38
4	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	37
5	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	37





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Operator : CG\JU
Sample : N2943-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

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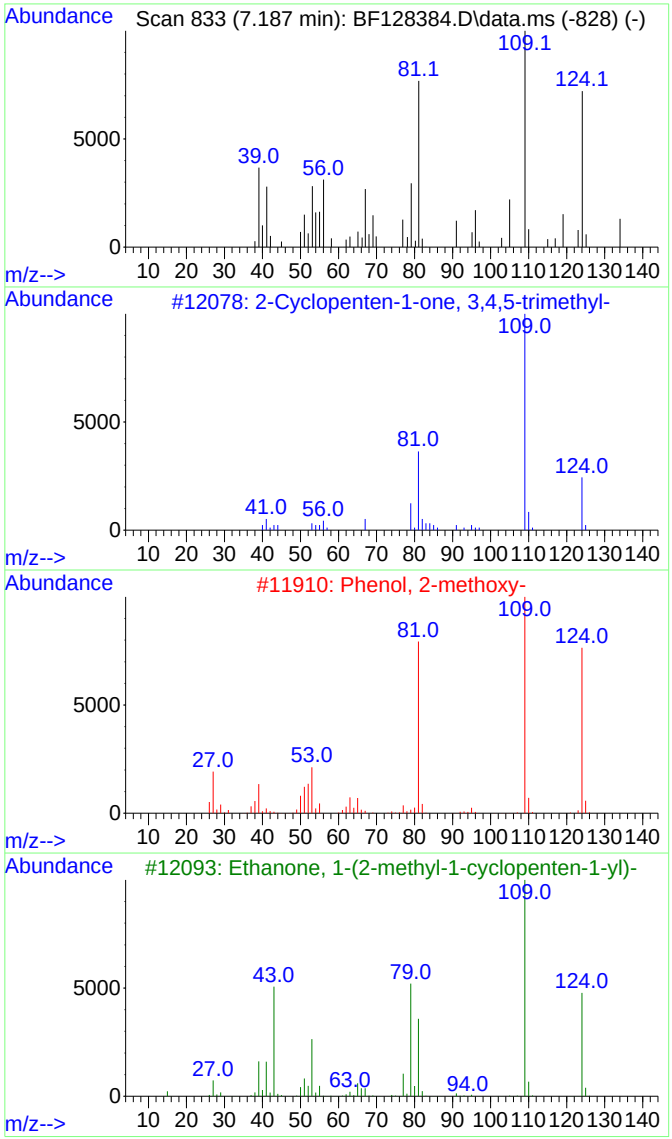
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

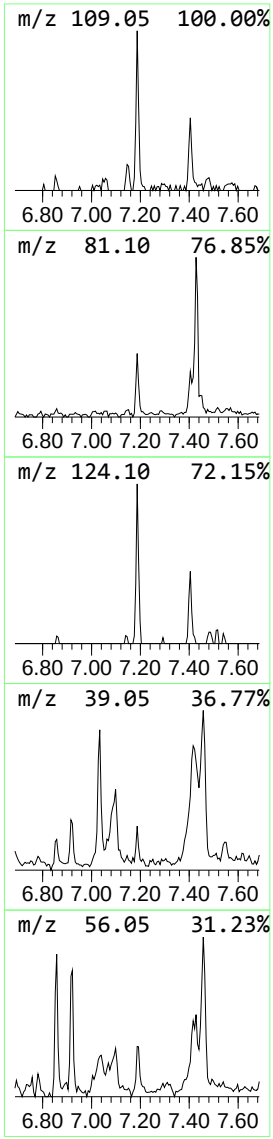
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Cyclopenten-1-one, 3,4,5-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.187	2.12 ng	57240	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	64
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	64
3	Ethanone, 1-(2-methyl-1-cyclopen...	124	C8H12O	003168-90-9	46
4	2,3,5-Trimethylcyclopent-2-enone	124	C8H12O	1000427-08-7	43
5	1,3-Pentadiene, 2,4-dimethyl-	96	C7H12	001000-86-8	38





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Operator : CG\JU
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Misc :
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Instrument :
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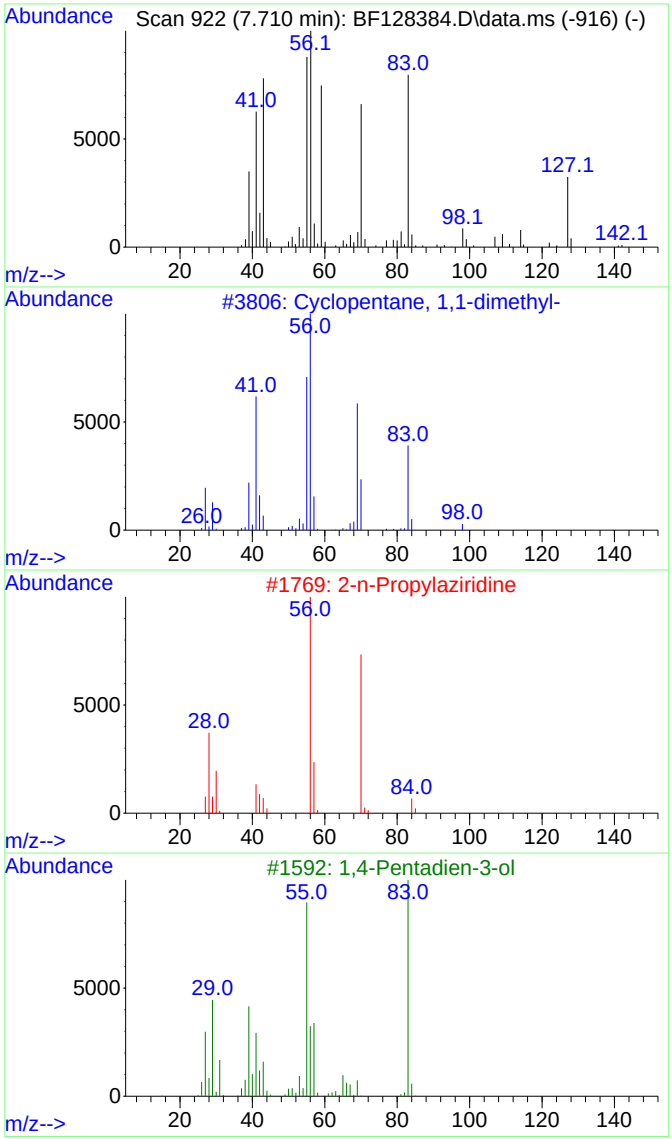
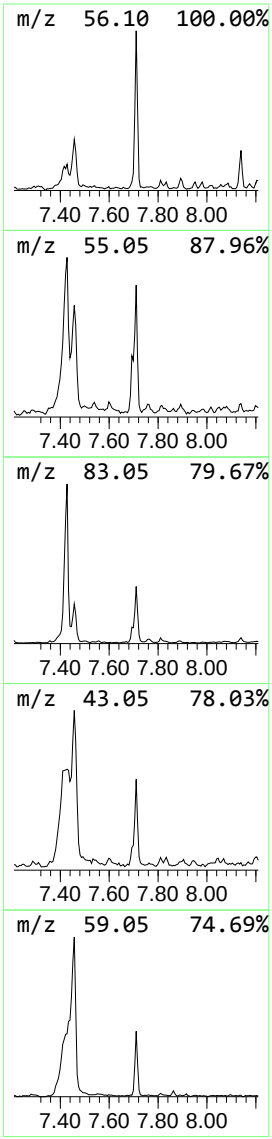
Peak Number 11 unknown7.710 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.710	5.02 ng	164543	Naphthalene-d8	8.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	43
2	2-n-Propylaziridine	85	C5H11N	003647-38-9	25
3	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	22
4	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	20
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	18





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

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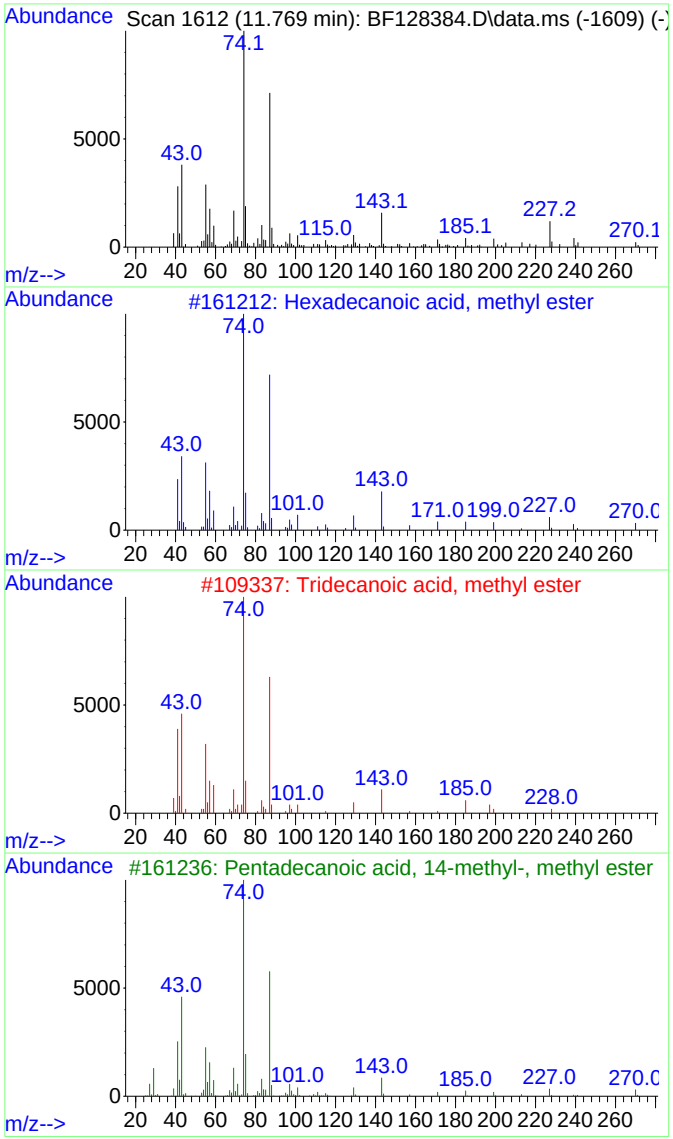
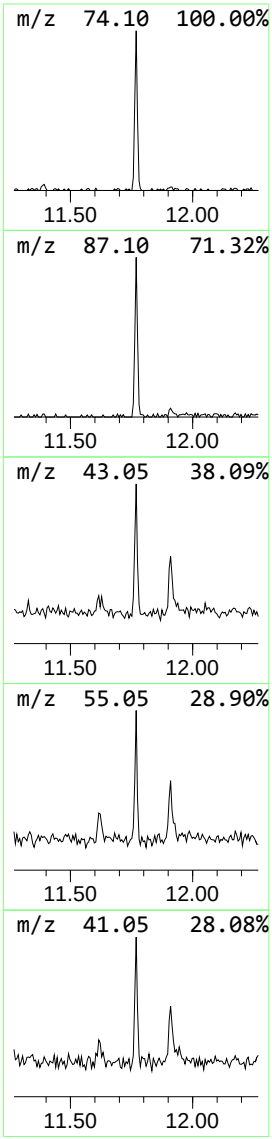
Peak Number 13 Hexadecanoic acid, methyl e... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.769	2.30 ng	74995	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	83
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	80
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	72





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Misc :
ALS Vial : 19 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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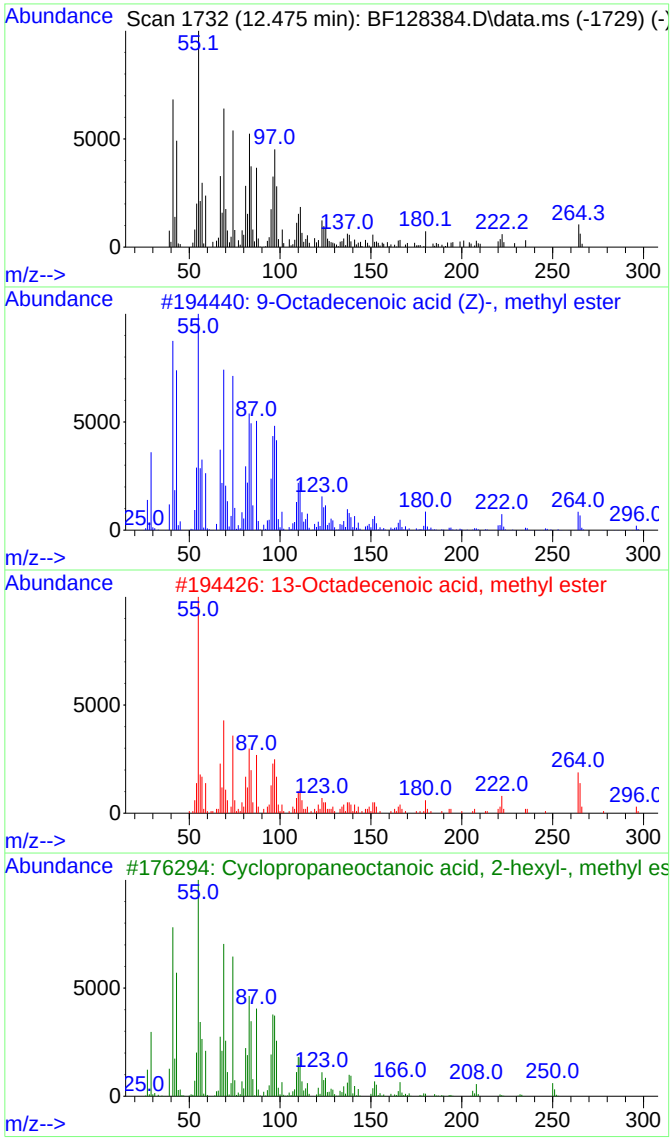
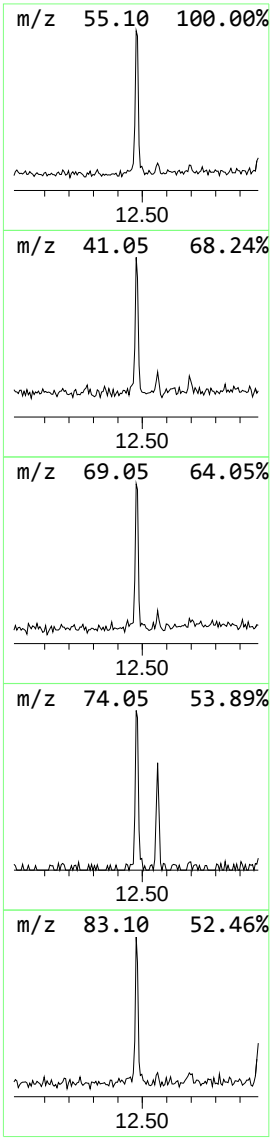
Peak Number 14 9-Octadecenoic acid (Z)-, m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	3.60 ng	117322	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
3	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87
4	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	87
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87





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TIC Library : C:\Database\NIST20.L
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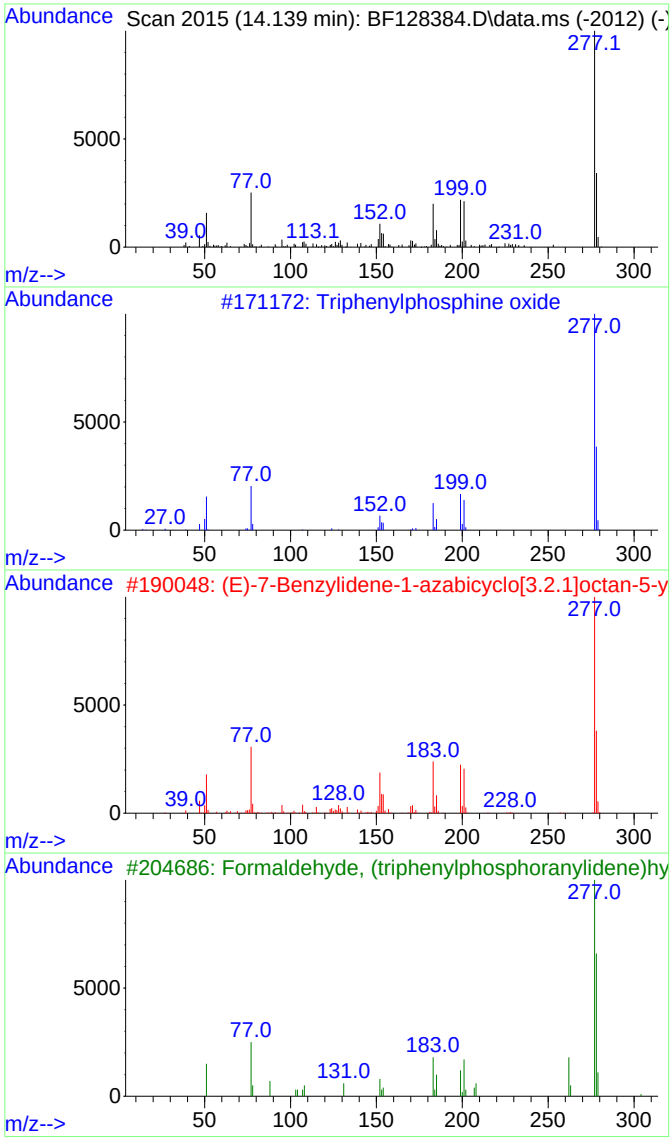
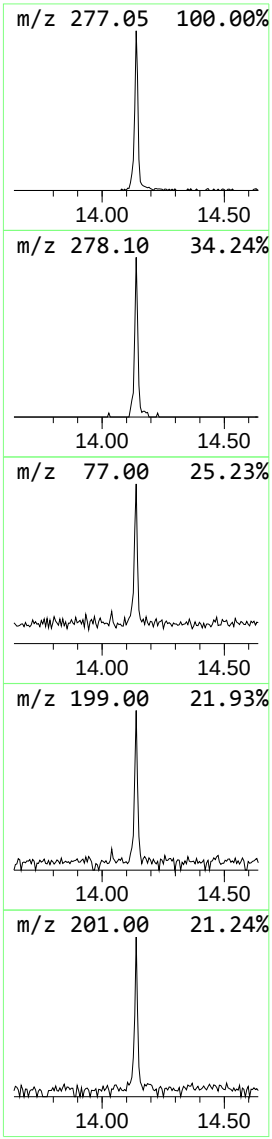
Peak Number 15 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.70 ng	62402	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	43
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32





Tentatively Identified Compound (LSC) summary

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BNA_F
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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-...	3.175	6.3	ng	170017	1	6.857	540042	20.0
Propane, 2-meth...	4.369	4.4	ng	118741	1	6.857	540042	20.0
unknown4.457	4.457	5.2	ng	140283	1	6.857	540042	20.0
Benzene, (1-met...	6.022	2.3	ng	60977	1	6.857	540042	20.0
unknown6.681	6.681	2.5	ng	66548	1	6.857	540042	20.0
1-Methyl-1H-1,2...	6.922	2.3	ng	60962	1	6.857	540042	20.0
Indane	7.034	12.4	ng	334132	1	6.857	540042	20.0
unknown7.098	7.098	9.4	ng	253546	1	6.857	540042	20.0
2-Cyclopenten-1...	7.187	2.1	ng	57240	1	6.857	540042	20.0
unknown7.710	7.710	5.0	ng	164543	2	8.140	655713	20.0
Hexadecanoic ac...	11.769	2.3	ng	74995	4	11.392	652678	20.0
9-Octadecenoic ...	12.475	3.6	ng	117322	4	11.392	652678	20.0
Triphenylphosph...	14.139	2.7	ng	62402	5	14.039	462333	20.0