LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127878.D
Acq On : 25 Apr 2022 14:04
Operator : CG\JU
Sample : N2481-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GES-1R

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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.275	334	338	342	rBV	111917	134632	2.35%	0.397%
2	4.481	368	373	381	rVB2	54405	75983	1.33%	0.224%
3	5.175	487	491	502	rBV	81861	98456	1.72%	0.290%
4	5.557	552	556	559	rBV	2395943	2218047	38.69%	6.536%
5	6.551	721	725	735	rBV	1417540	1443613	25.18%	4.254%
6	6.739	753	757	759	rBV	106614	104275	1.82%	0.307%
7	6.763	759	761	771	rVB	105426	130764	2.28%	0.385%
8	6.857	774	777	787	rBV	135171	181567	3.17%	0.535%
9	6.939	787	791	794	rBV	1176367	948051	16.54%	2.794%
10	6.998	798	801	804	rBV	80187	109731	1.91%	0.323%
11	7.339	854	859	869	rVB3	42687	67339	1.17%	0.198%
12	7.504	878	887	890	rBV	3073628	3384982	59.05%	9.975%
13	7.575	895	899	902	rVV	63799	66522	1.16%	0.196%
14	8.222	1005	1009	1012	rBV	1475380	1276505	22.27%	3.762%
15	8.451	1038	1048	1050	rBV4	23922	76621	1.34%	0.226%
16	8.551	1061	1065	1071	rBV5	38728	68936	1.20%	0.203%
17	8.633	1074	1079	1089	rVB	88535	116207	2.03%	0.342%
18	9.216	1172	1178	1186	rBV3	74183	174138	3.04%	0.513%
19	9.298	1186	1192	1196	rBV	5249445	5665612	98.83%	16.695%
20	9.398	1205	1209	1225	rVB	2523264	2577070	44.95%	7.594%
21	9.980	1299	1308	1311	rBV	1812809	1533883	26.76%	4.520%
22	10.392	1374	1378	1382	rVB	170500	147882	2.58%	0.436%
23	10.680	1424	1427	1430	rBV	204898	166373	2.90%	0.490%
24	10.774	1438	1443	1446	rBV	3593009	3522242	61.44%	10.379%
25	11.474	1558	1562	1565	rBV	1752915	1557836	27.17%	4.591%
26	11.851	1623	1626	1629	rBV	230362	171672	2.99%	0.506%
27	13.063	1827	1832	1836	rBV	5077804	5732735	100.00%	16.893%
28	14.115	2007	2011	2018	rBV	1243468	1115253	19.45%	3.286%
29	14.210	2023	2027	2036	rBV	88843	113238	1.98%	0.334%
30	15.633	2263	2269	2279	rBV	680566	955546	16.67%	2.816%

Sum of corrected areas: 33935711

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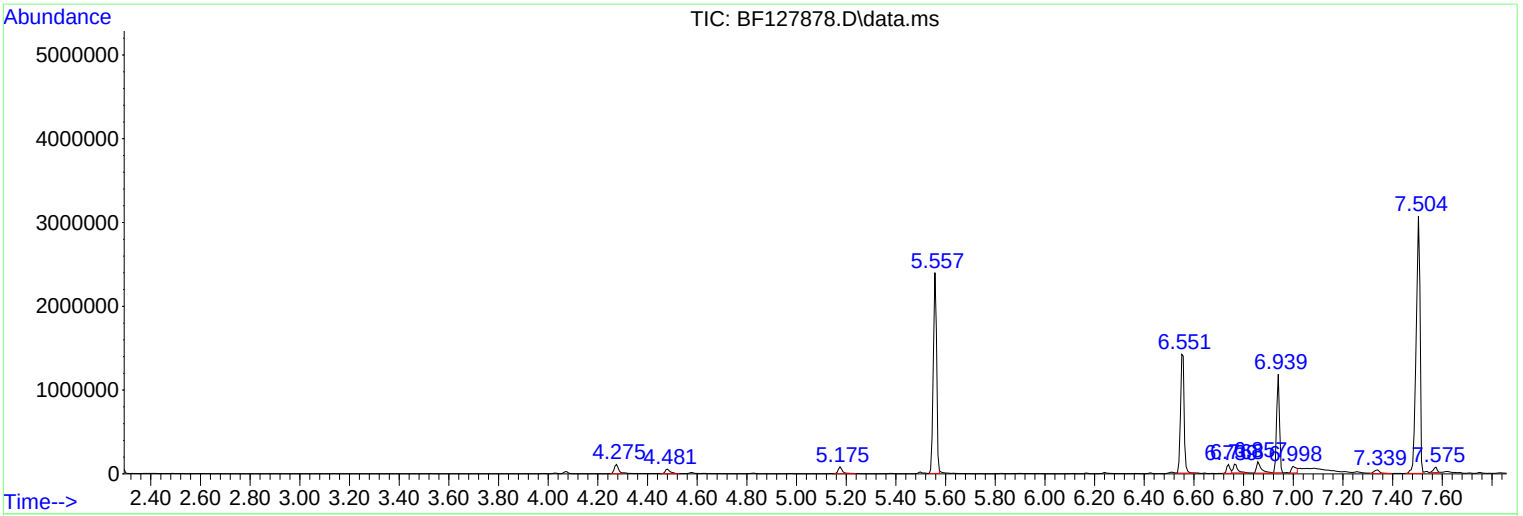
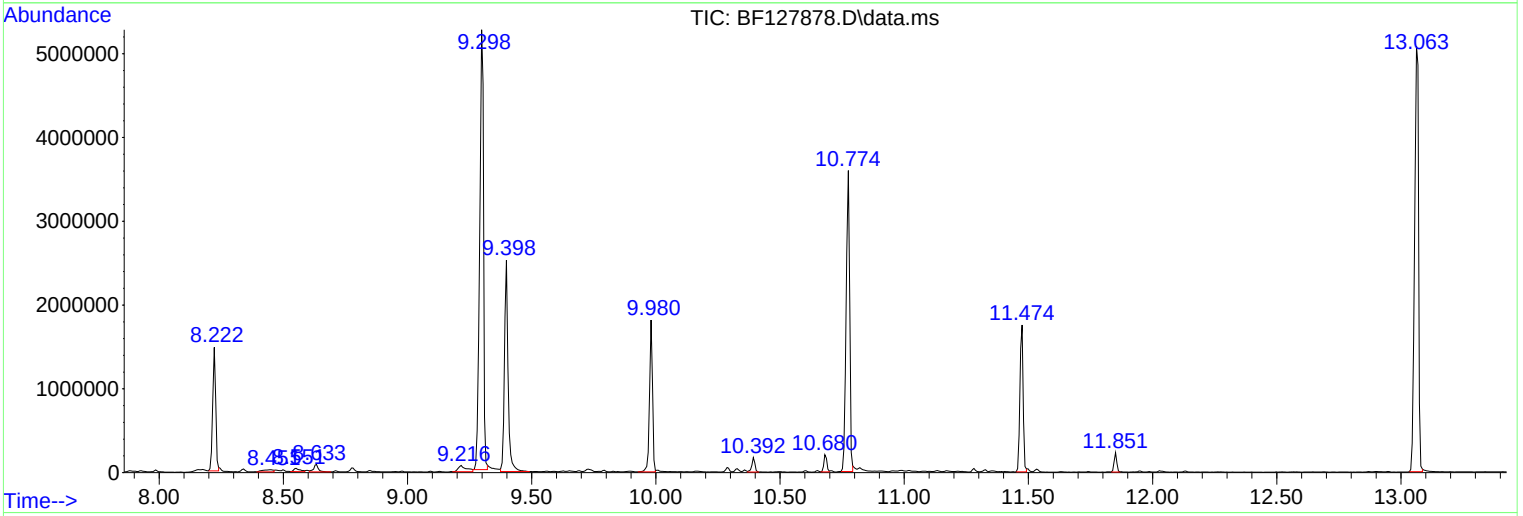
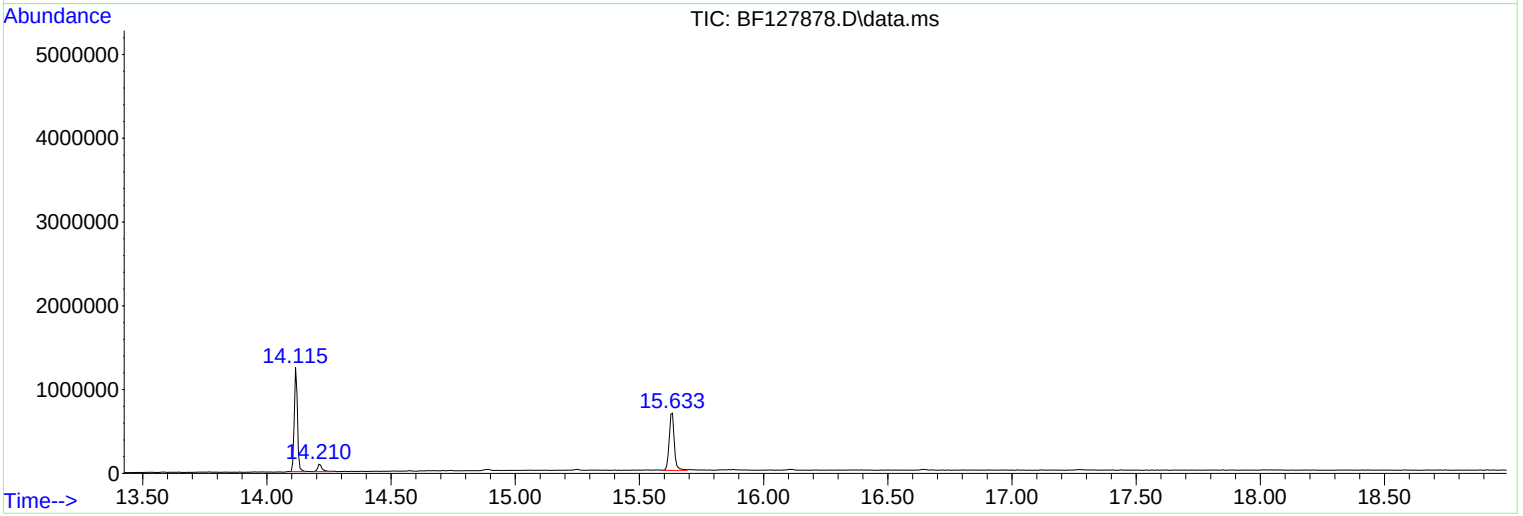
Instrument :
BNA_F
ClientSampleId :
GES-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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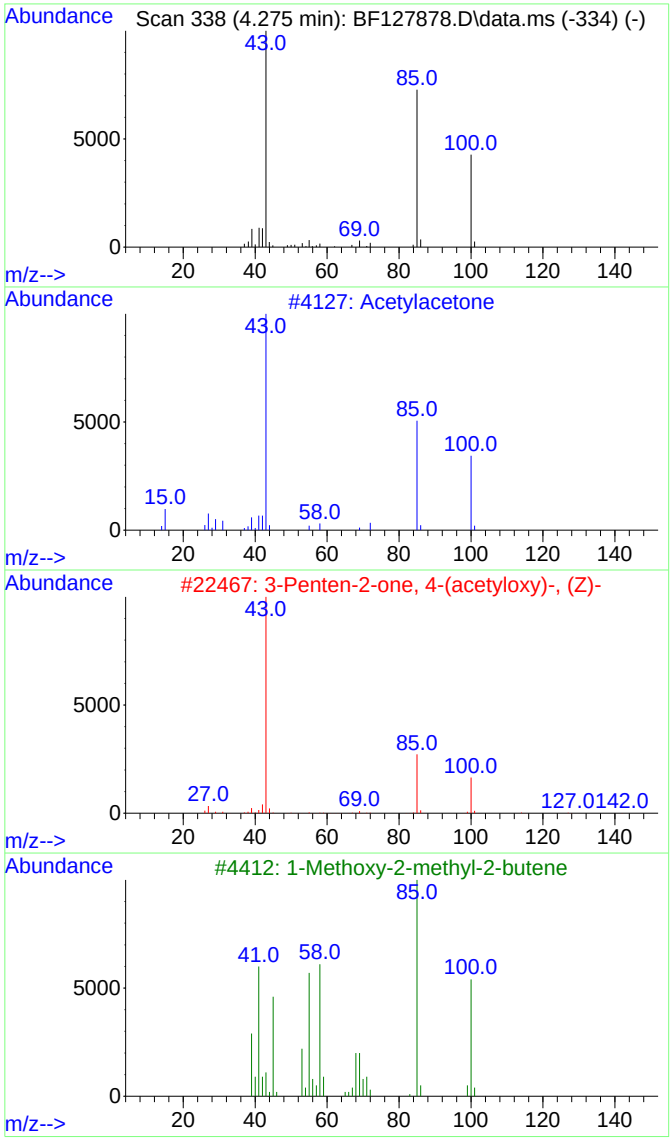
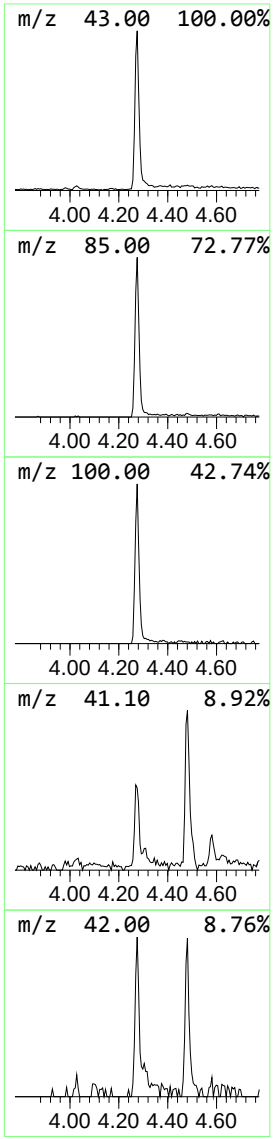
****

Peak Number 1 Acetylacetone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.275	2.84 ng	134632	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetylacetone	100	C5H8O2	000123-54-6	86
2	3-Penten-2-one, 4-(acetyloxy)-, ...	142	C7H10O3	038365-58-1	78
3	1-Methoxy-2-methyl-2-butene	100	C6H12O	1000279-59-7	59
4	Propionaldehyde, ethylhydrazone	100	C5H12N2	007422-92-6	45
5	Hexane, 2-bromo-	164	C6H13Br	003377-86-4	43





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
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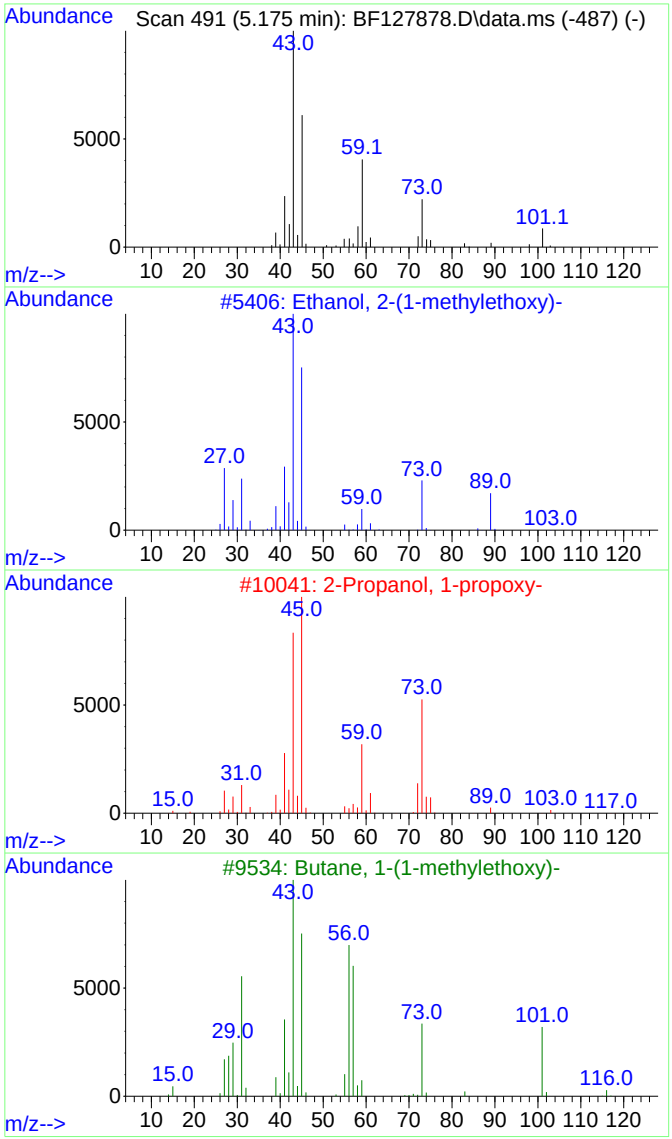
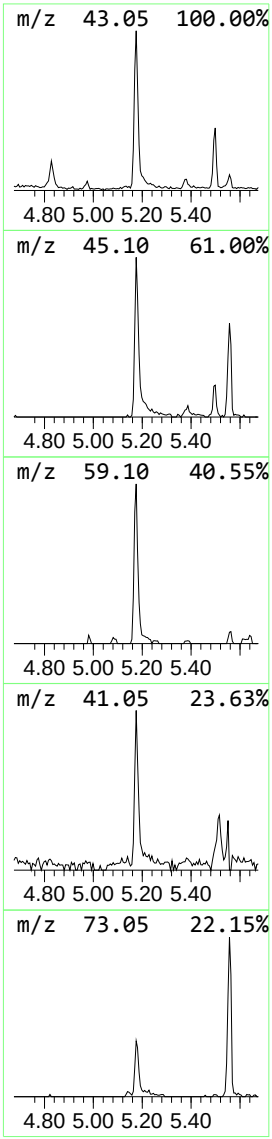
****

Peak Number 2 unknown5.175 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	2.08 ng	98456	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	47
2	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	43
3	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	40
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
5	Diacetamide	101	C4H7NO2	000625-77-4	38





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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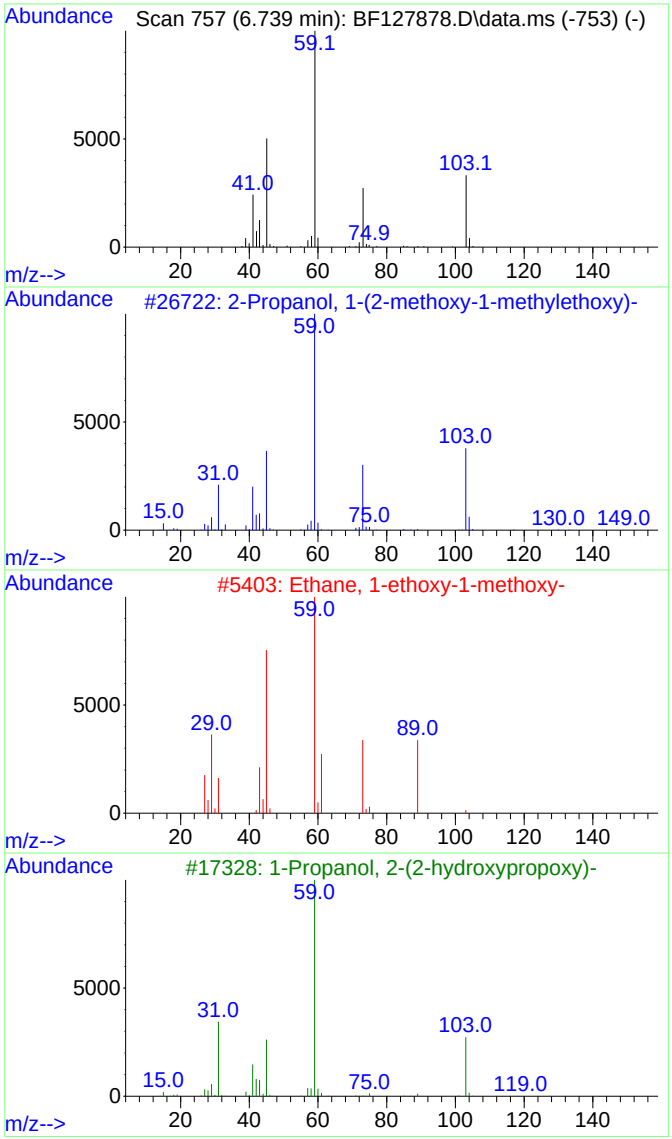
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

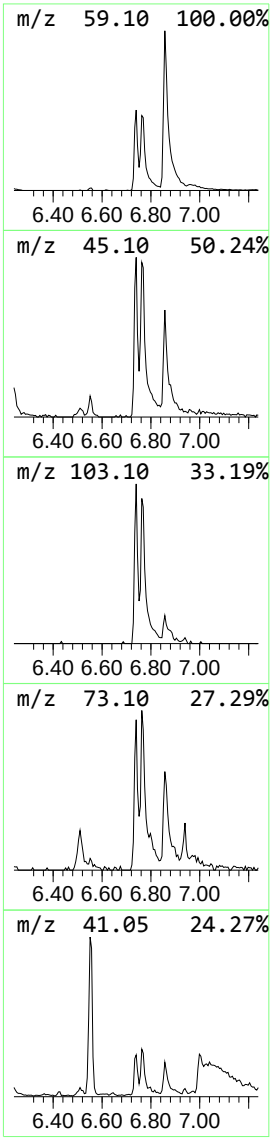
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.739	2.20 ng	104275	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	42
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	40
5	Ethyl ether	74	C4H10O	000060-29-7	38





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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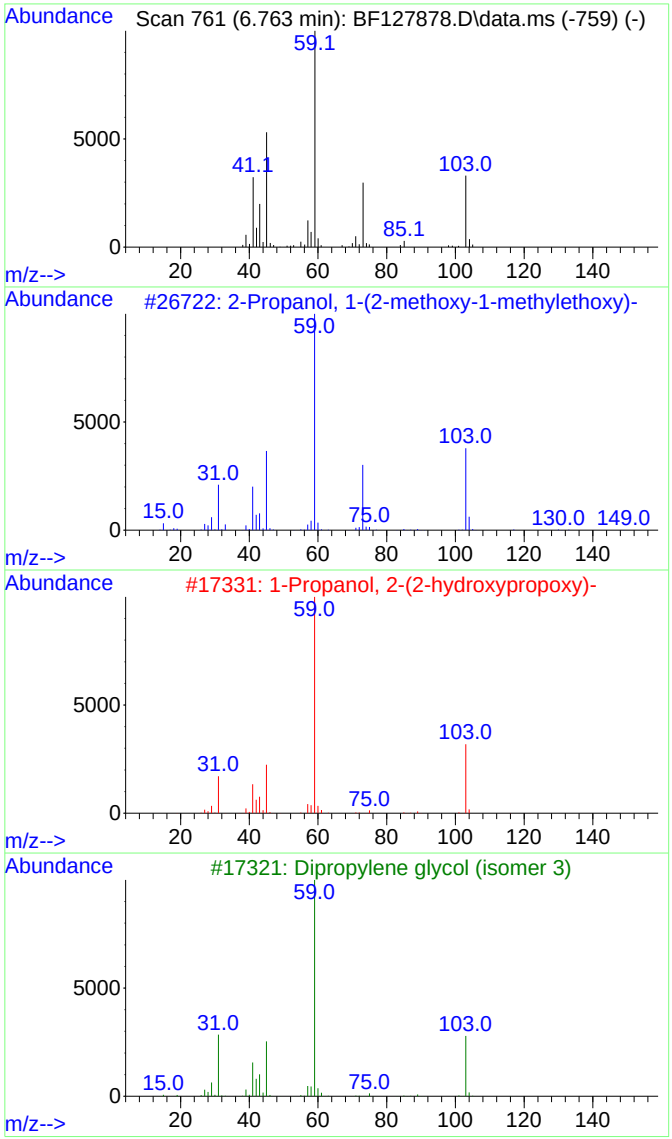
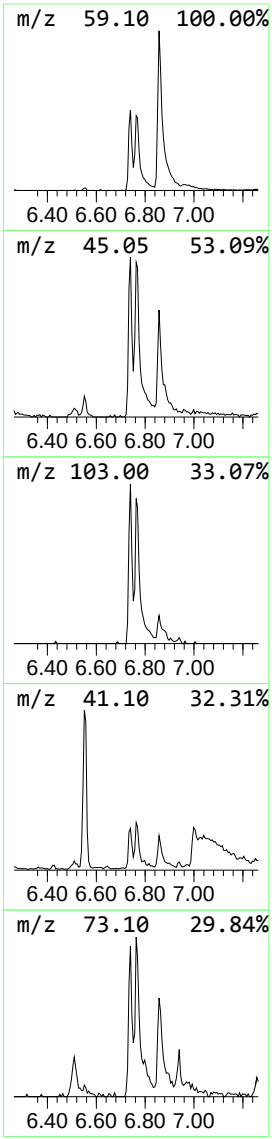
****
Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.763	2.76 ng	130764	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	50
5	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	45





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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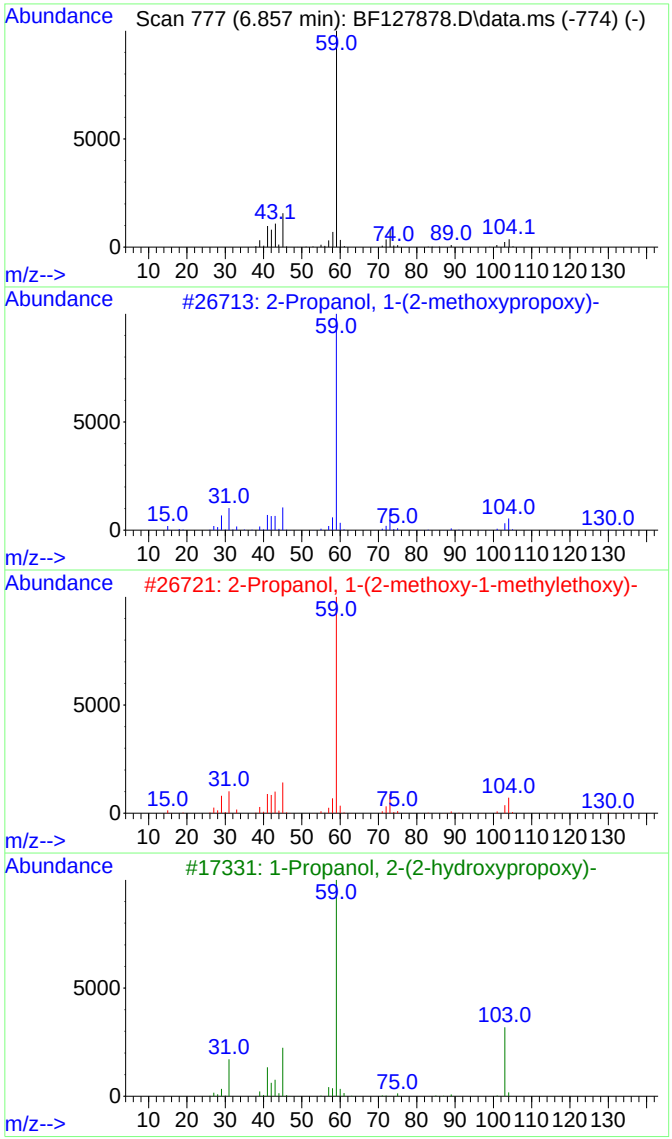
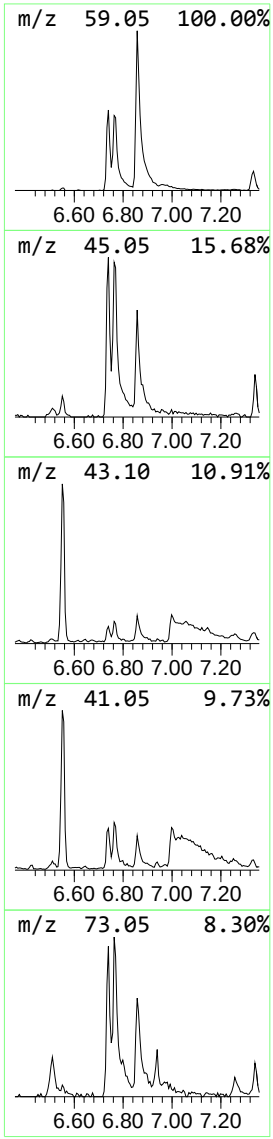
****
Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.857	3.83 ng	181567	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





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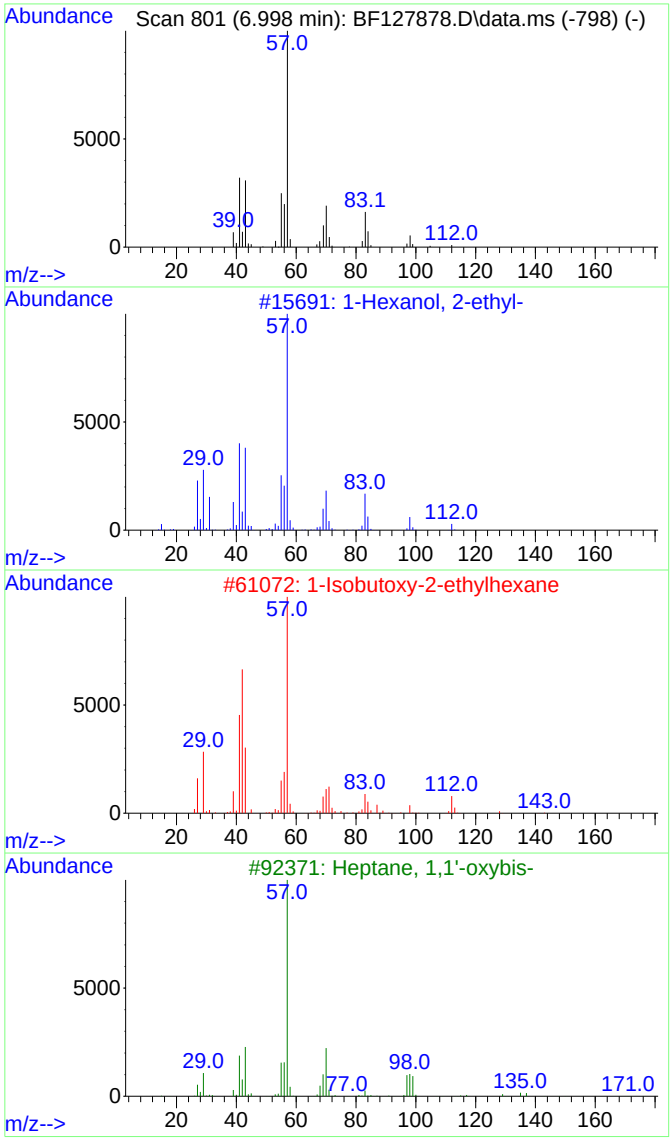
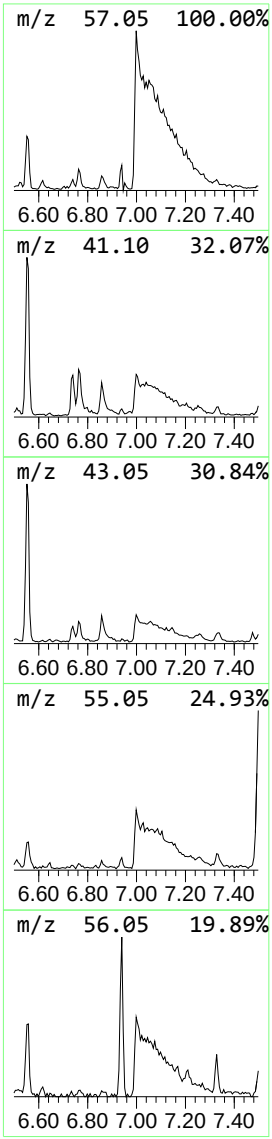
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.998	2.31 ng	109731	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	78
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	59
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53





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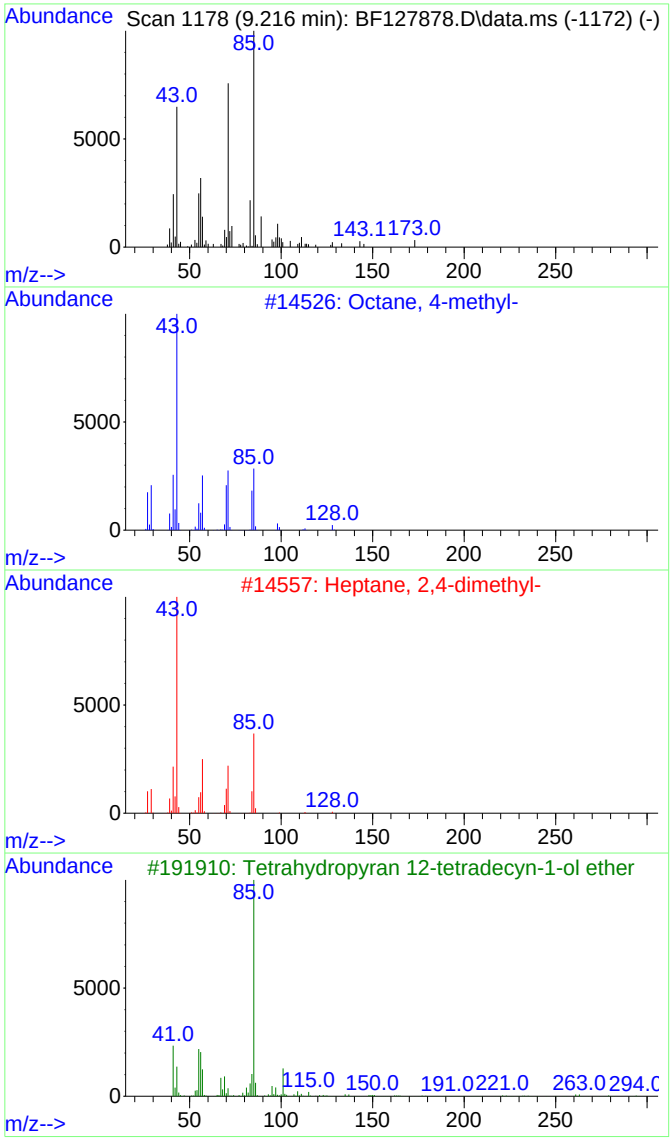
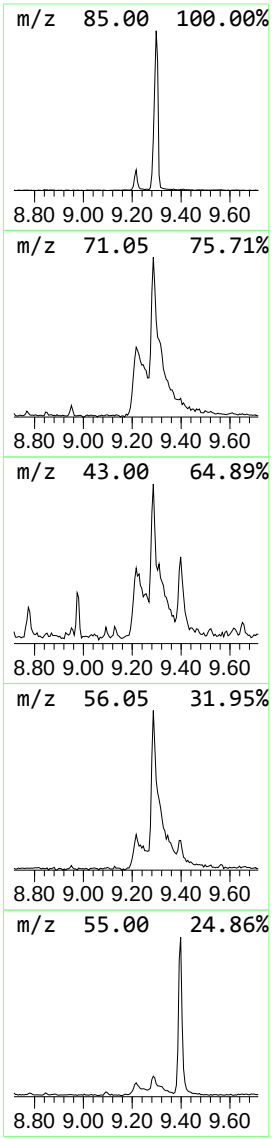
****

Peak Number 7 Octane, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	2.27 ng	174138	Acenaphthene-d10	9.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	59
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	38
3	Tetrahydropyran 12-tetradecyn-1-...	294	C19H34O2	096249-40-0	35
4	2H-Pyran, tetrahydro-2-[(2-nitro...	259	C13H25NO4	1000188-29-8	35
5	2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	35





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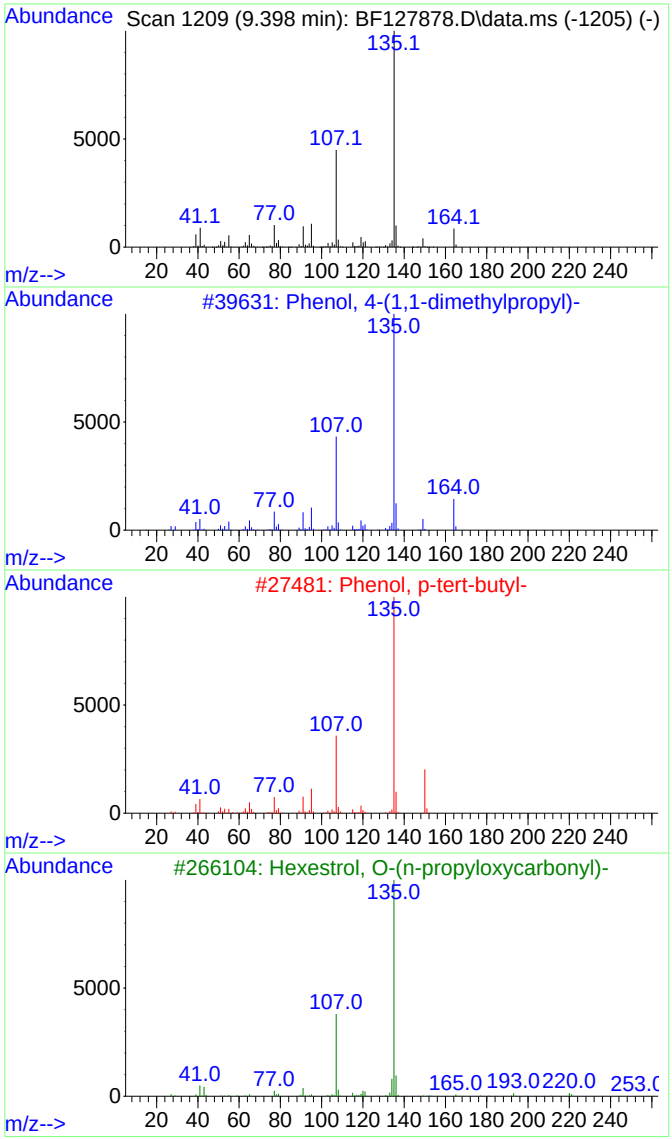
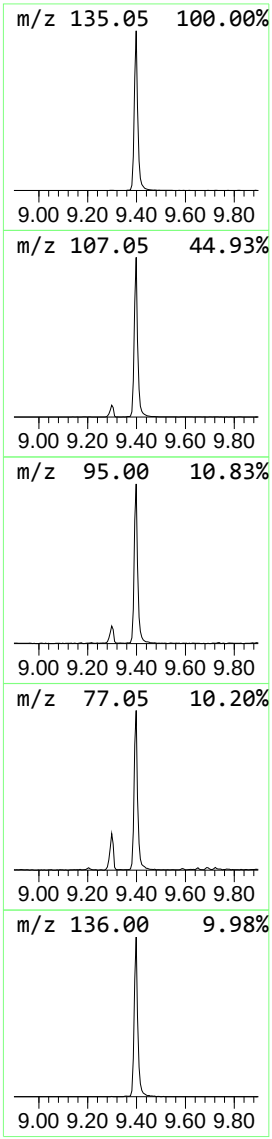
****
Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.398	33.60 ng	2577070	Acenaphthene-d10	9.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	64
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
5	Hexestrol, O-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64





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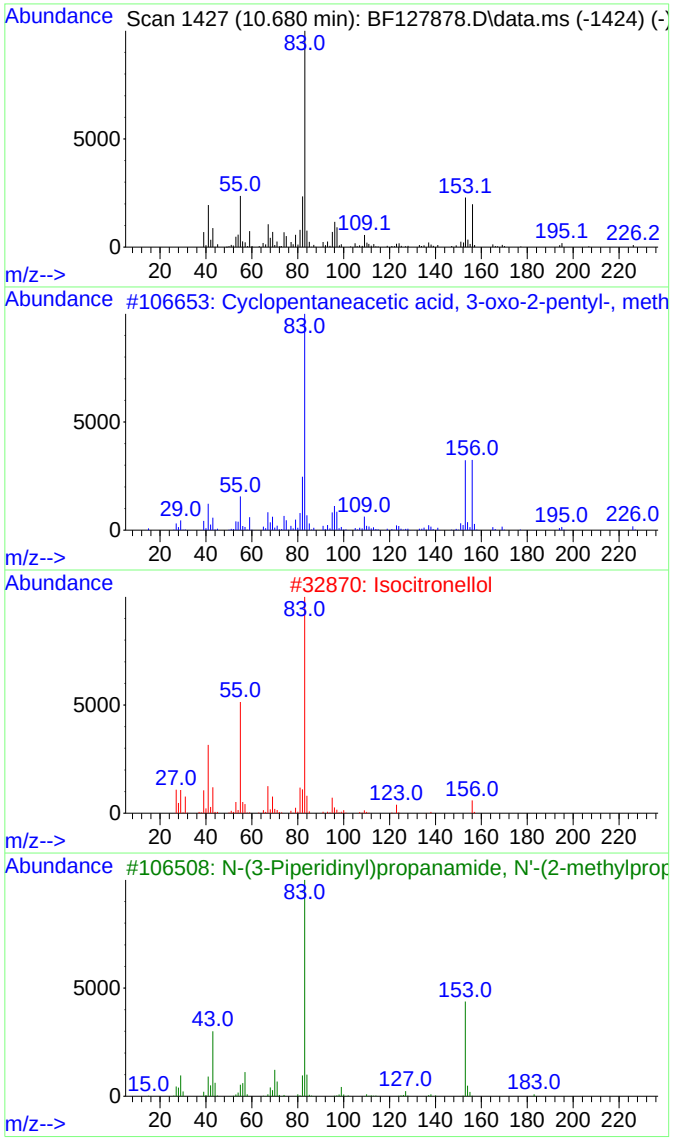
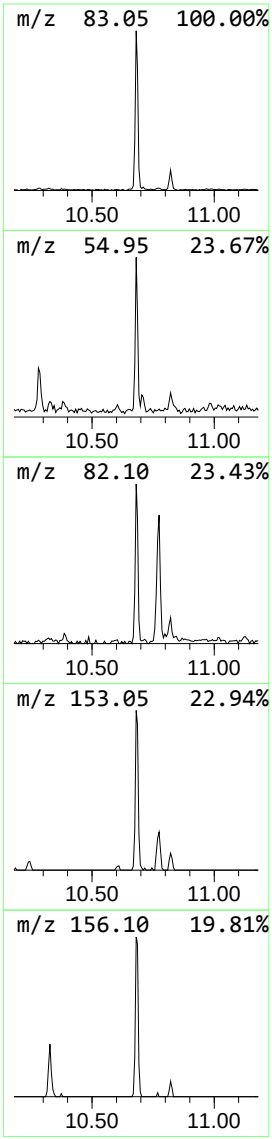
****
Peak Number 9 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.680	2.17 ng	166373	Acenaphthene-d10	9.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	96
2	Isocitronellol	156	C10H20O	018479-52-2	50
3	N-(3-Piperidinyl)propanamide, N'...	226	C12H22N2O2	1000469-85-0	47
4	2-Nonen-4-one, 2-methyl-	154	C10H18O	002903-23-3	38
5	Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	38





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Data File : BF127878.D
Acq On : 25 Apr 2022 14:04
Operator : CG\JU
Sample : N2481-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GES-1R

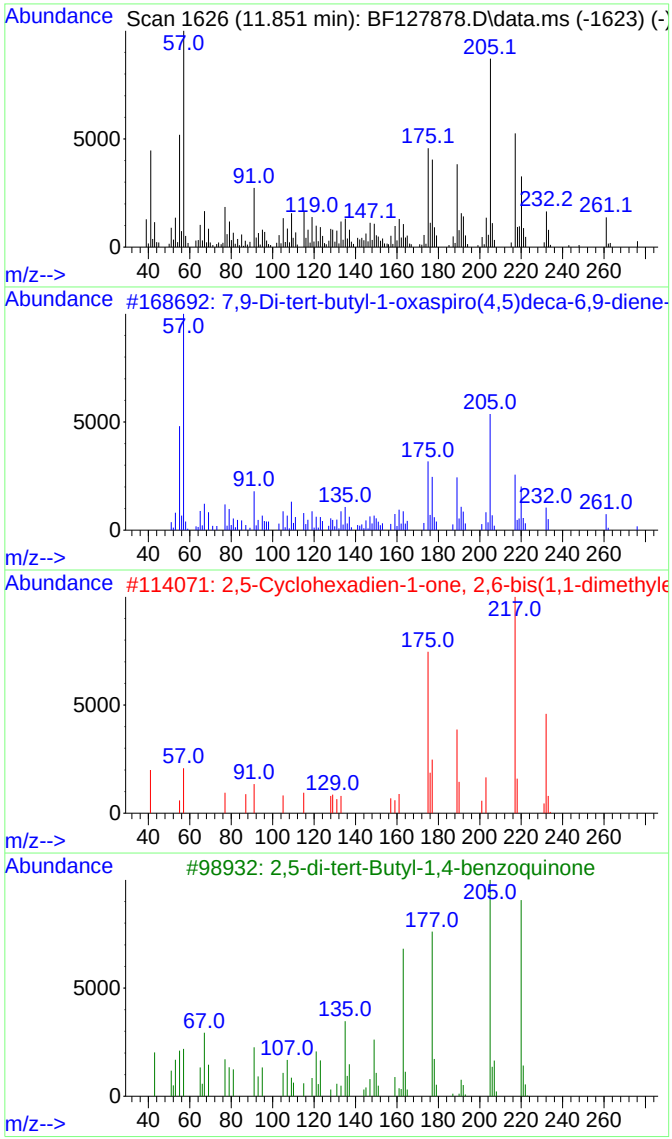
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

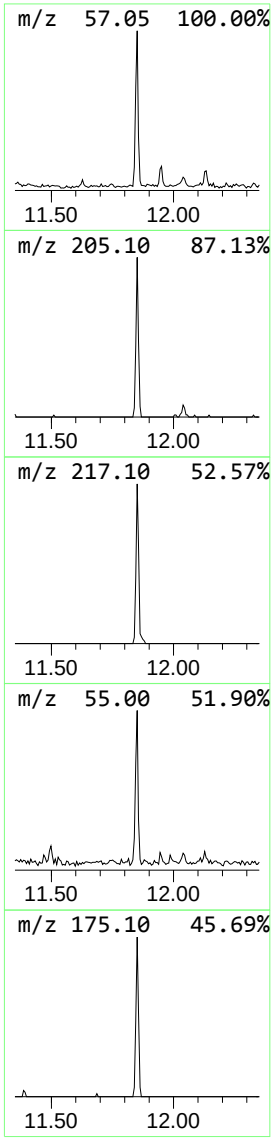
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.20 ng	171672	Phenanthrene-d10	11.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	83
3	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	50
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	45
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127878.D
Acq On : 25 Apr 2022 14:04
Operator : CG\JU
Sample : N2481-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GES-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

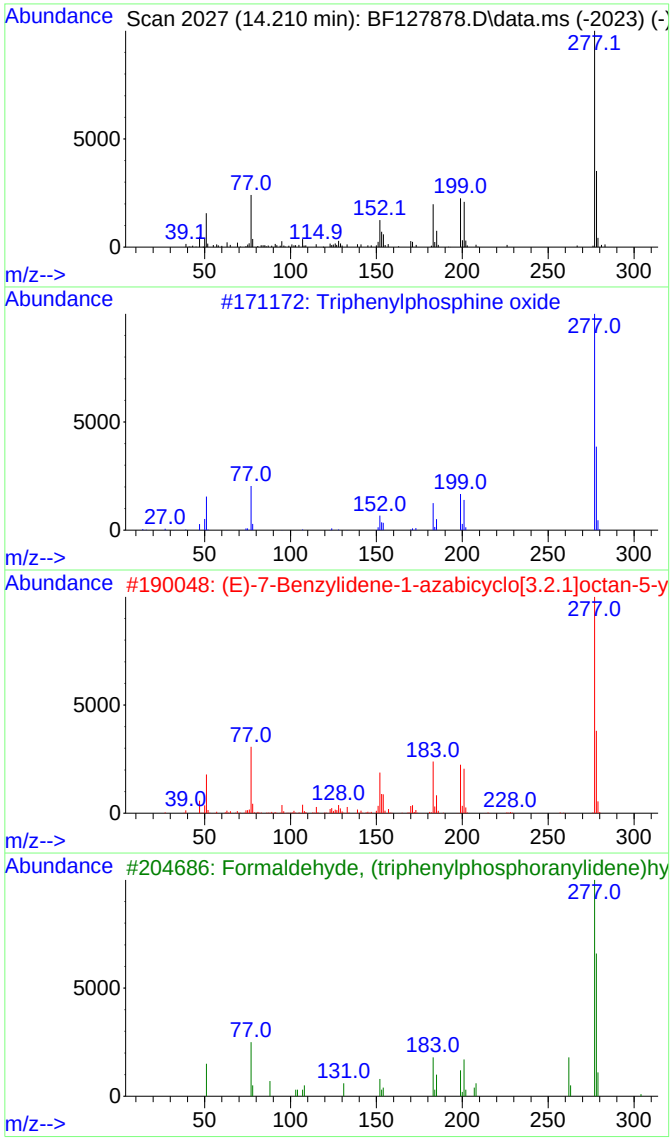
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

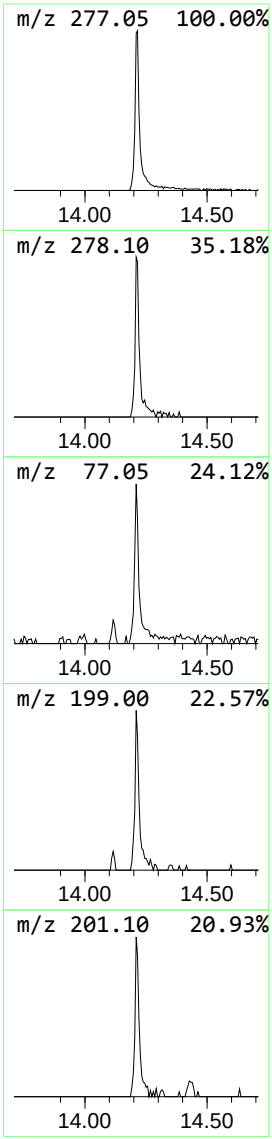
****

Peak Number 11 Triphenylphosphine oxide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	2.03 ng	113238	Chrysene-d12	14.115

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
4	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
5	5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127878.D
Acq On : 25 Apr 2022 14:04
Operator : CG\JU
Sample : N2481-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GES-1R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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
Acetylacetone	4.275	2.8	ng	134632	1	6.939	948051	20.0
unknown5.175	5.175	2.1	ng	98456	1	6.939	948051	20.0
2-Propanol, 1-(...	6.739	2.2	ng	104275	1	6.939	948051	20.0
1-Propanol, 2-(...	6.763	2.8	ng	130764	1	6.939	948051	20.0
2-Propanol, 1-(...	6.857	3.8	ng	181567	1	6.939	948051	20.0
1-Hexanol, 2-et...	6.998	2.3	ng	109731	1	6.939	948051	20.0
Octane, 4-methyl-	9.216	2.3	ng	174138	3	9.980	1533880	20.0
Phenol, 4-(1,1-...	9.398	33.6	ng	2577070	3	9.980	1533880	20.0
Cyclopentaneace...	10.680	2.2	ng	166373	3	9.980	1533880	20.0
7,9-Di-tert-but...	11.851	2.2	ng	171672	4	11.474	1557840	20.0
Triphenylphosph...	14.210	2.0	ng	113238	5	14.115	1115250	20.0