LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
Data File : BF127953.D
Acq On : 27 Apr 2022 18:59
Operator : CG\JU
Sample : N2482-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-9

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: BF127953.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.469	367	371	383	rVV2	277899	409572	9.49%	1.754%
2	4.569	383	388	393	rVB	96524	107697	2.49%	0.461%
3	5.169	485	490	501	rBV	105986	130988	3.03%	0.561%
4	5.551	549	555	559	rBV	2198967	2098581	48.62%	8.985%
5	6.104	645	649	652	rBV	176943	137331	3.18%	0.588%
6	6.392	694	698	701	rBV	176687	141603	3.28%	0.606%
7	6.551	720	725	734	rBV	1606050	1610483	37.31%	6.895%
8	6.728	751	755	757	rBV	109074	107192	2.48%	0.459%
9	6.757	757	760	770	rVV	104427	176199	4.08%	0.754%
10	6.845	772	775	786	rVV	117924	236605	5.48%	1.013%
11	6.928	786	789	796	rVB	700661	664682	15.40%	2.846%
12	7.110	813	820	823	rBV	317162	287291	6.66%	1.230%
13	7.334	853	858	868	rVB2	68457	97448	2.26%	0.417%
14	7.498	881	886	889	rVB	2478947	2593050	60.07%	11.102%
15	7.881	946	951	958	rBV3	64669	70600	1.64%	0.302%
16	7.945	958	962	965	rVV	53809	49233	1.14%	0.211%
17	8.151	992	997	1000	rBV	89011	97406	2.26%	0.417%
18	8.210	1003	1007	1011	rBV	842648	785407	18.19%	3.363%
19	8.328	1023	1027	1031	rBV	38933	45629	1.06%	0.195%
20	8.616	1073	1076	1083	rVB2	37330	51968	1.20%	0.223%
21	9.204	1171	1176	1178	rBV3	47320	60797	1.41%	0.260%
22	9.292	1185	1191	1194	rBV	4261968	4316720	100.00%	18.482%
23	9.386	1204	1207	1224	rVB	848563	1041786	24.13%	4.460%
24	9.969	1298	1306	1310	rBV	965378	847347	19.63%	3.628%
25	10.380	1372	1376	1379	rVB	174598	148482	3.44%	0.636%
26	10.674	1423	1426	1428	rBV	142465	123891	2.87%	0.530%
27	10.763	1437	1441	1444	rBV	2272814	2010772	46.58%	8.609%
28	11.463	1556	1560	1567	rBV	850602	705832	16.35%	3.022%
29	11.839	1621	1624	1627	rBV	101580	76947	1.78%	0.329%
30	13.051	1825	1830	1833	rBV	3374234	2918419	67.61%	12.495%
31	14.110	2006	2010	2018	rVB	556436	538870	12.48%	2.307%
32	15.615	2261	2266	2272	rBV2	519988	667518	15.46%	2.858%

Sum of corrected areas: 23356346

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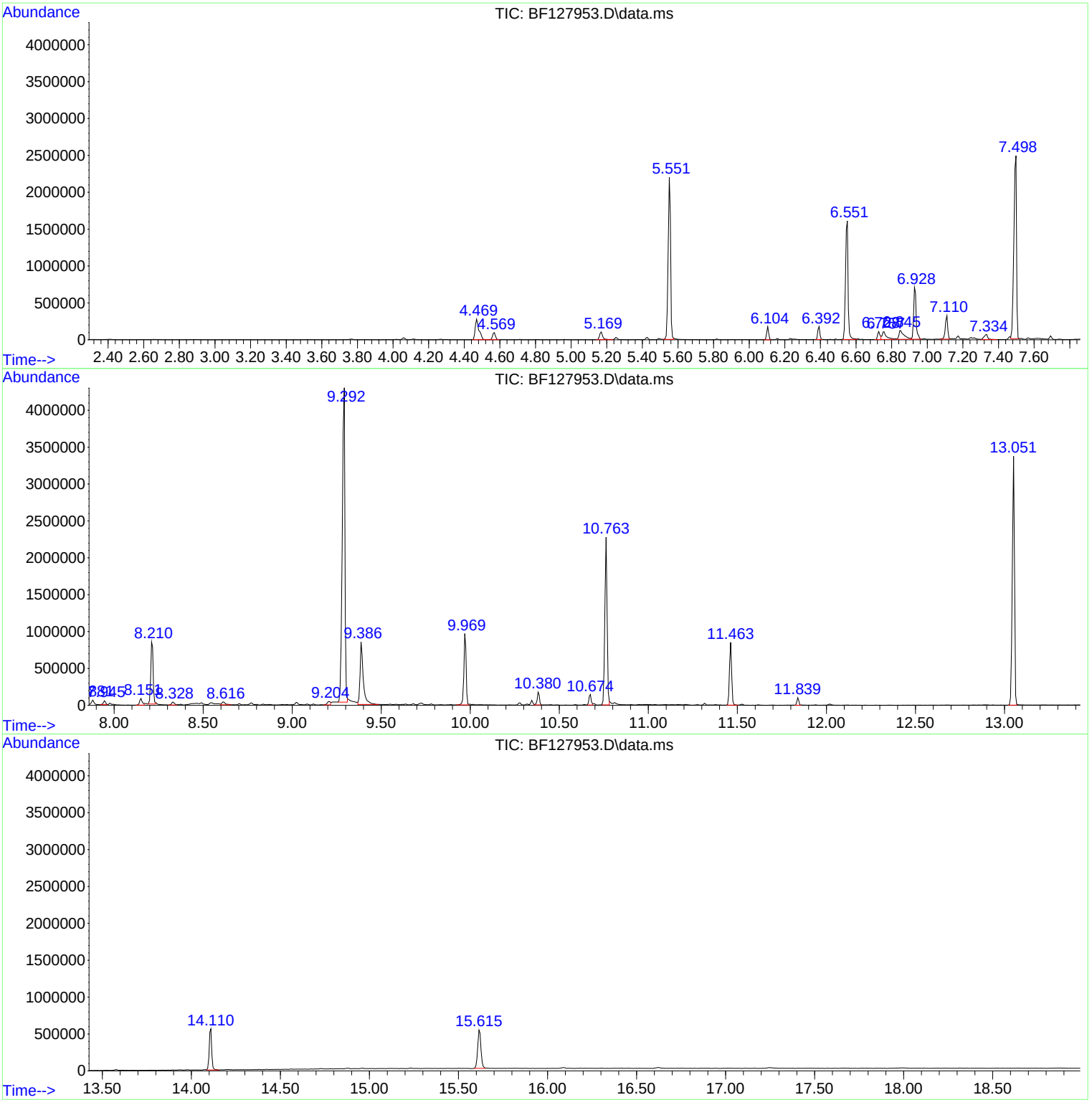
Instrument :
BNA_F
ClientSampleId :
SPN-9

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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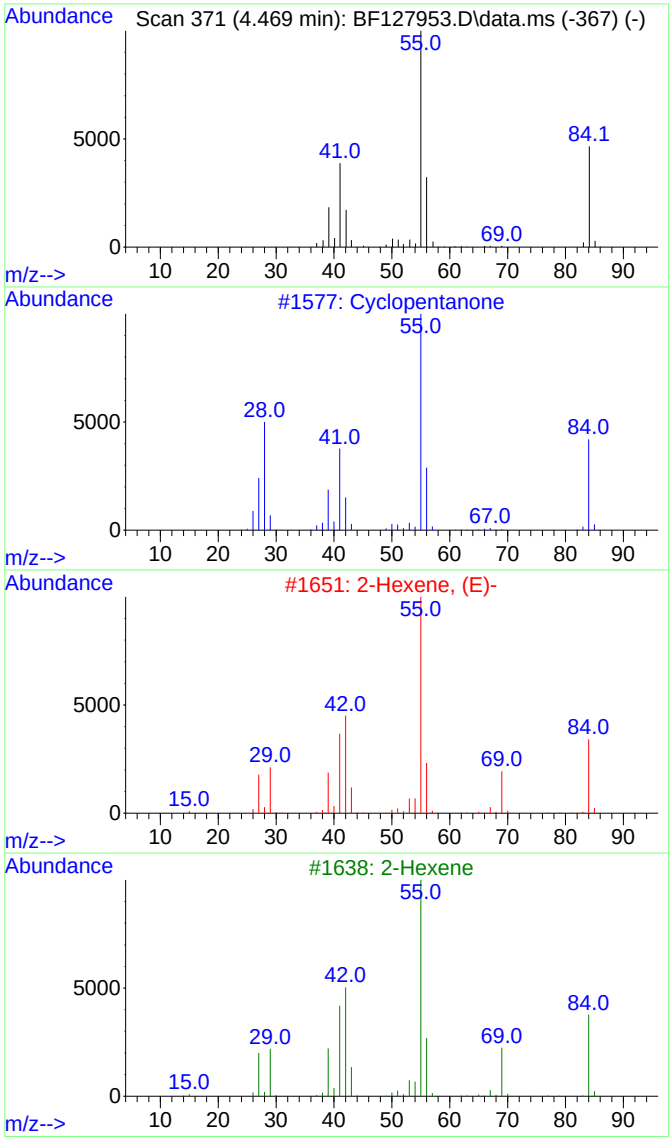
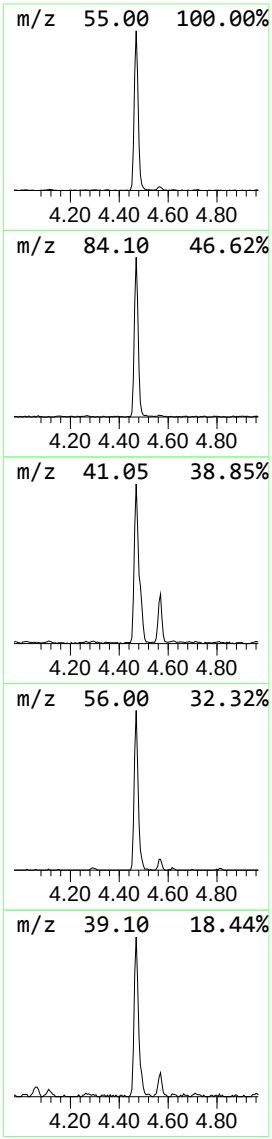
Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.469	12.32 ng	409572	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	90
2	2-Hexene, (E)-	84	C6H12	004050-45-7	50
3	2-Hexene	84	C6H12	000592-43-8	50
4	3-Hexene	84	C6H12	000592-47-2	50
5	3-Hexene, (Z)-	84	C6H12	007642-09-3	50





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Data File : BF127953.D
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Operator : CG\JU
Sample : N2482-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-9

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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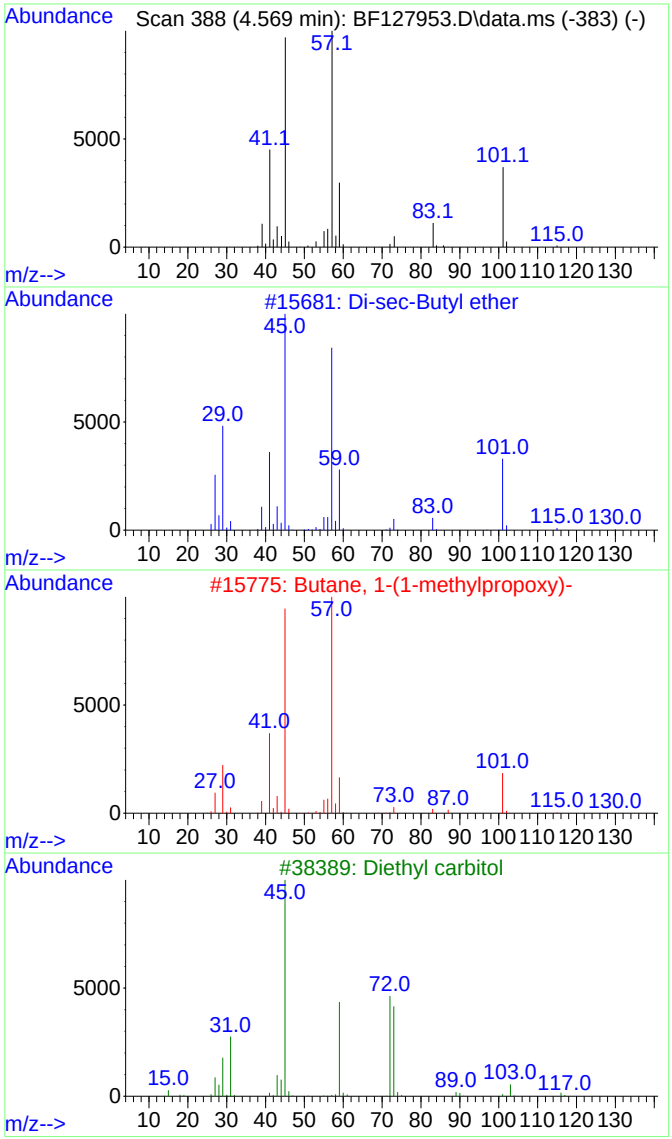
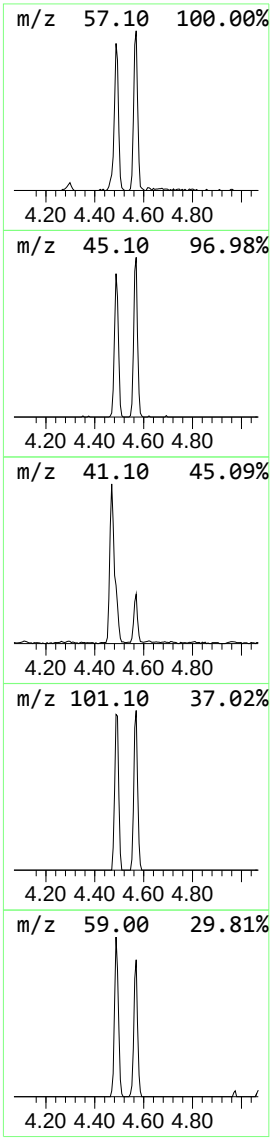
Peak Number 2 Di-sec-Butyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.569	3.24 ng	107697	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	80
3	Diethyl carbitol	162	C8H18O3	000112-36-7	50
4	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	40
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40





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Operator : CG\JU
Sample : N2482-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
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

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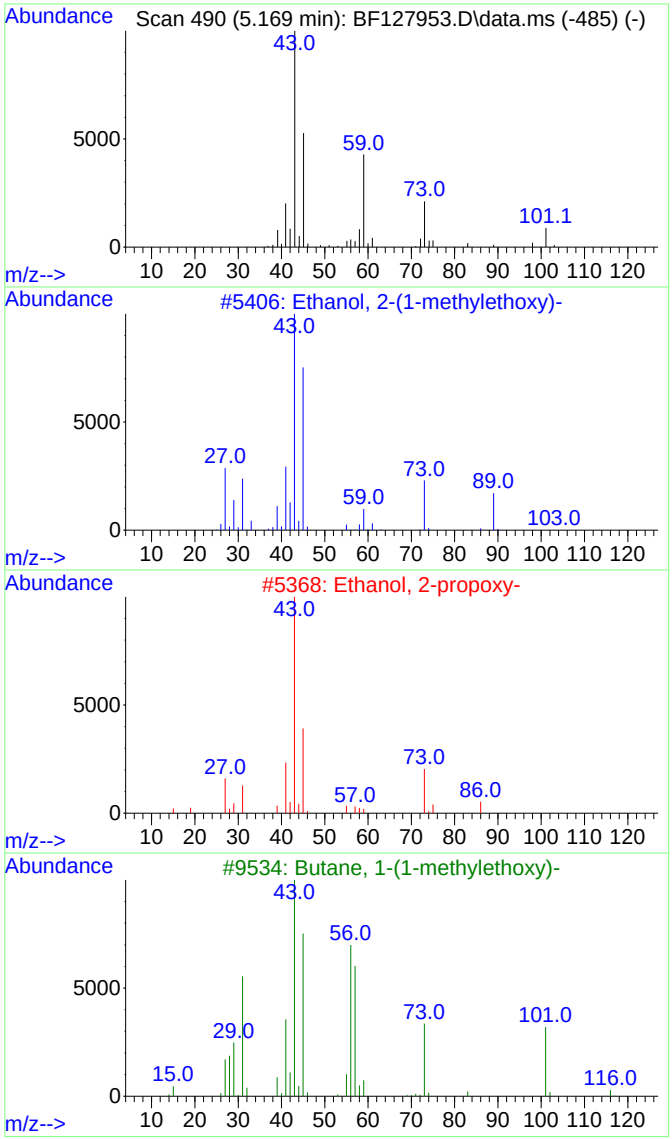
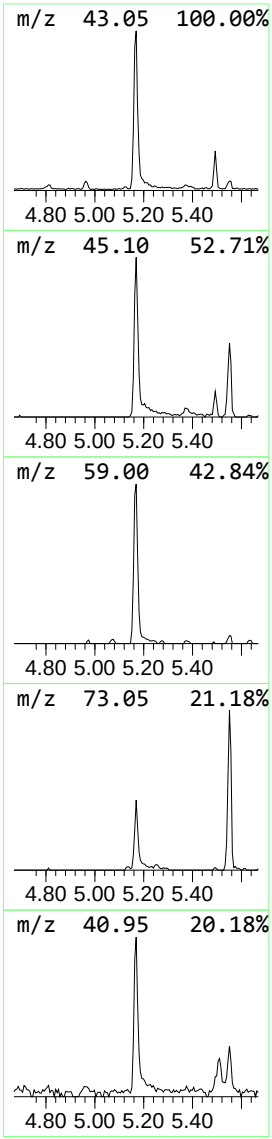
Peak Number 3 unknown5.169 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	3.94 ng	130988	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	43
2	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	38
3	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	38
4	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	38
5	2,3-Epoxybutane	72	C4H8O	003266-23-7	35





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
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

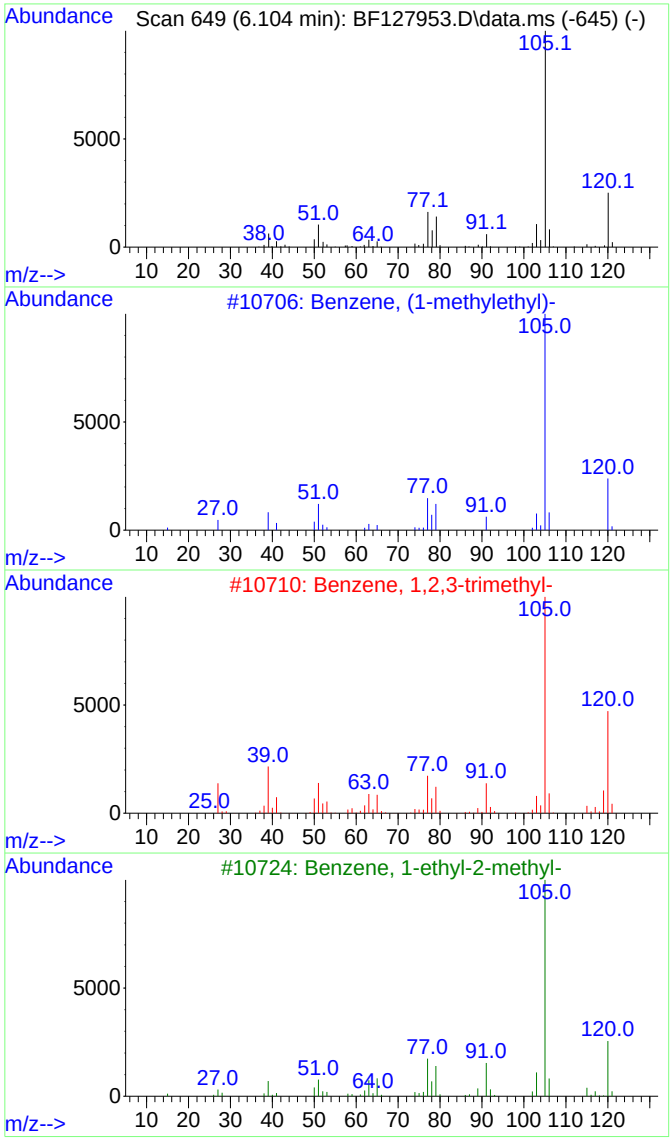
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

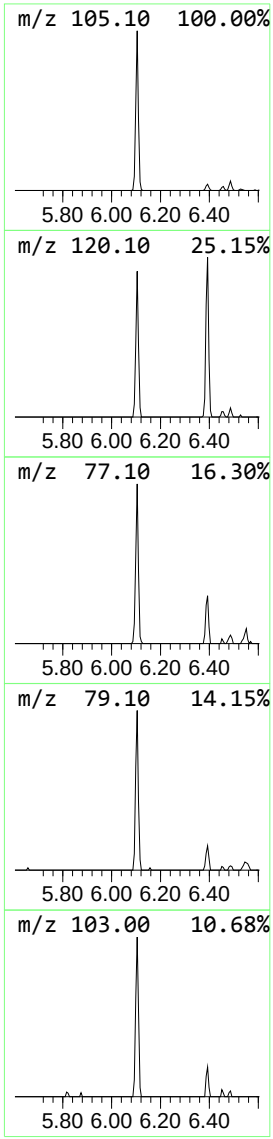
****

Peak Number 4 Benzene, (1-methylethyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.104	4.13 ng	137331	1,4-Dichlorobenzene-d4	6.934

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-2-methyl-	120	C9H12	000611-14-3	83
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	80
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	80





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Sample : N2482-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
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
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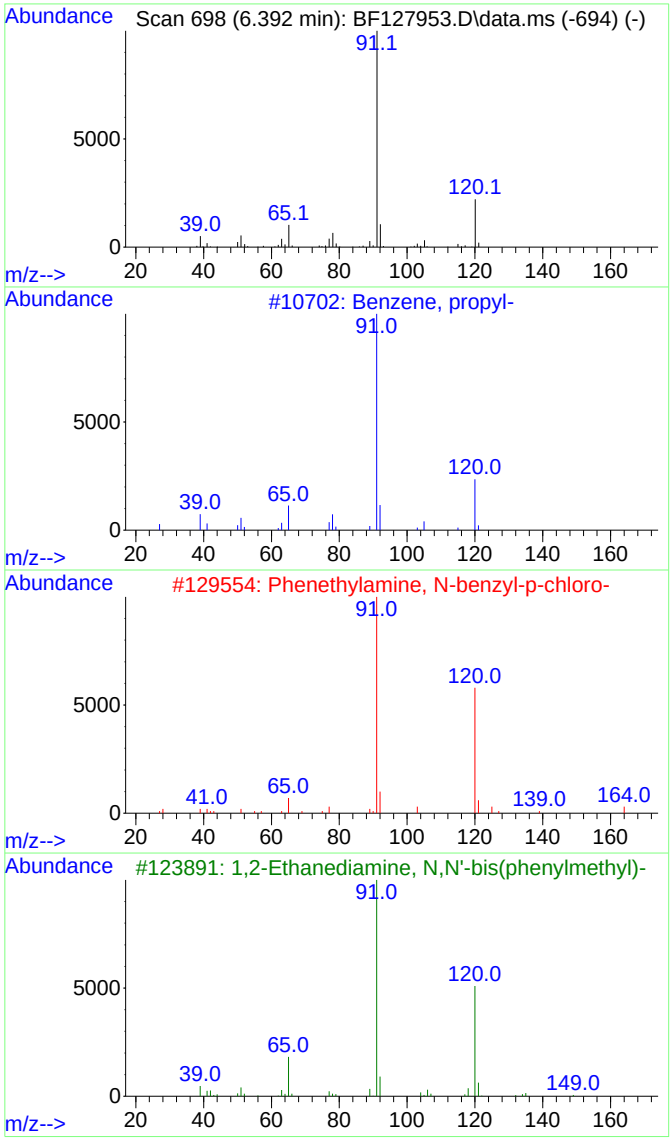
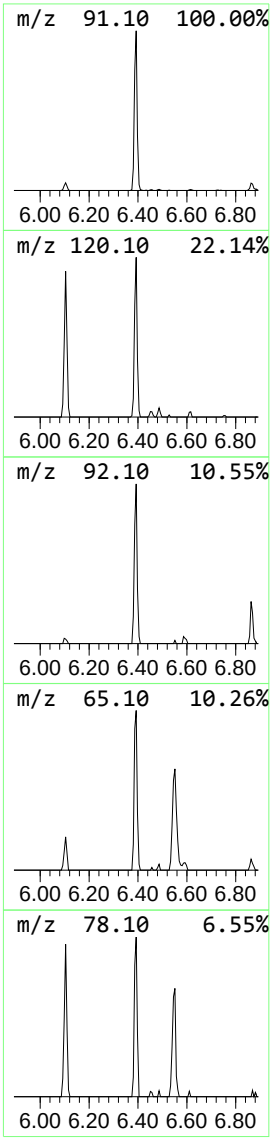
****

Peak Number 5 Benzene, propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.392	4.26 ng	141603	1,4-Dichlorobenzene-d4	6.934

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	1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	72
4	N-Isobutyl(phenyl)methanesulfona...	227	C11H17NO2S	144615-94-1	64
5	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	64





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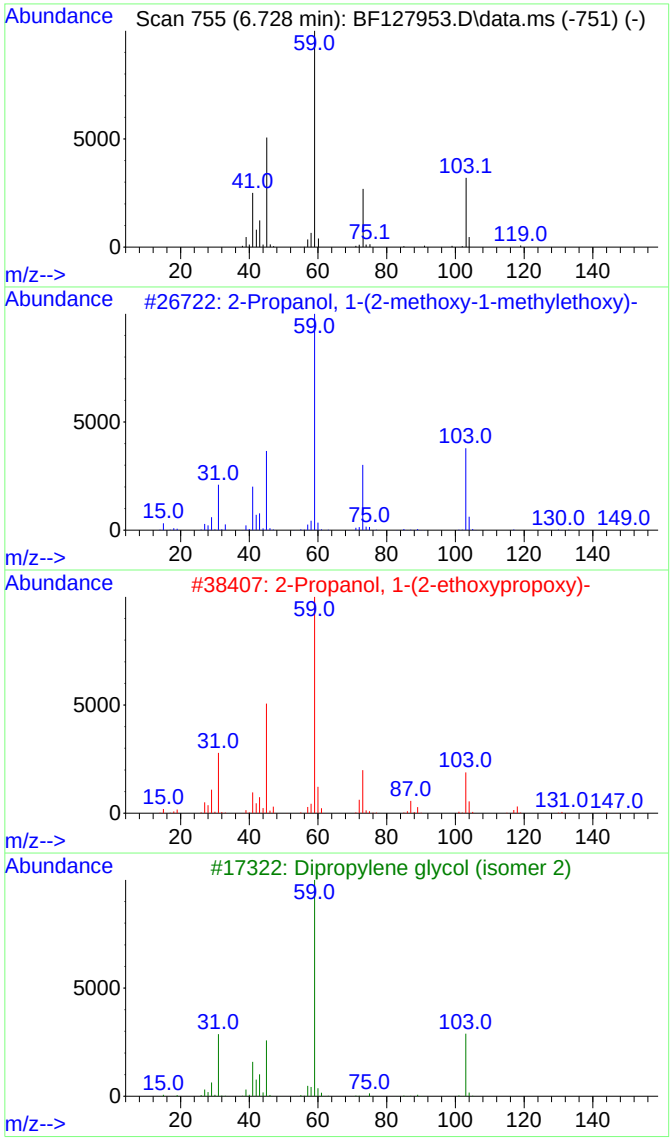
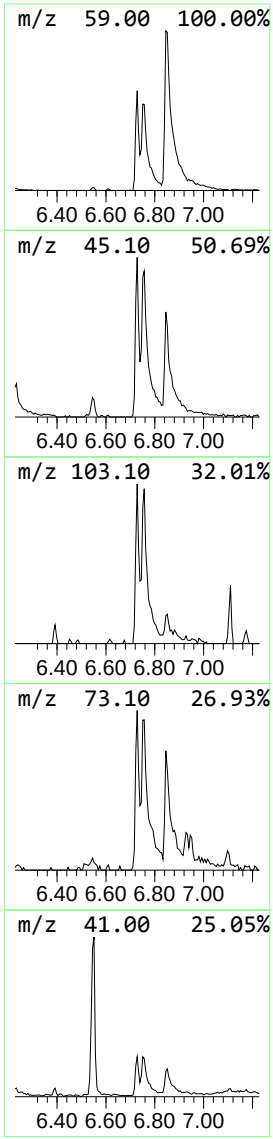
****
Peak Number 6 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	3.23 ng	107192	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	80
2	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	72
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
5	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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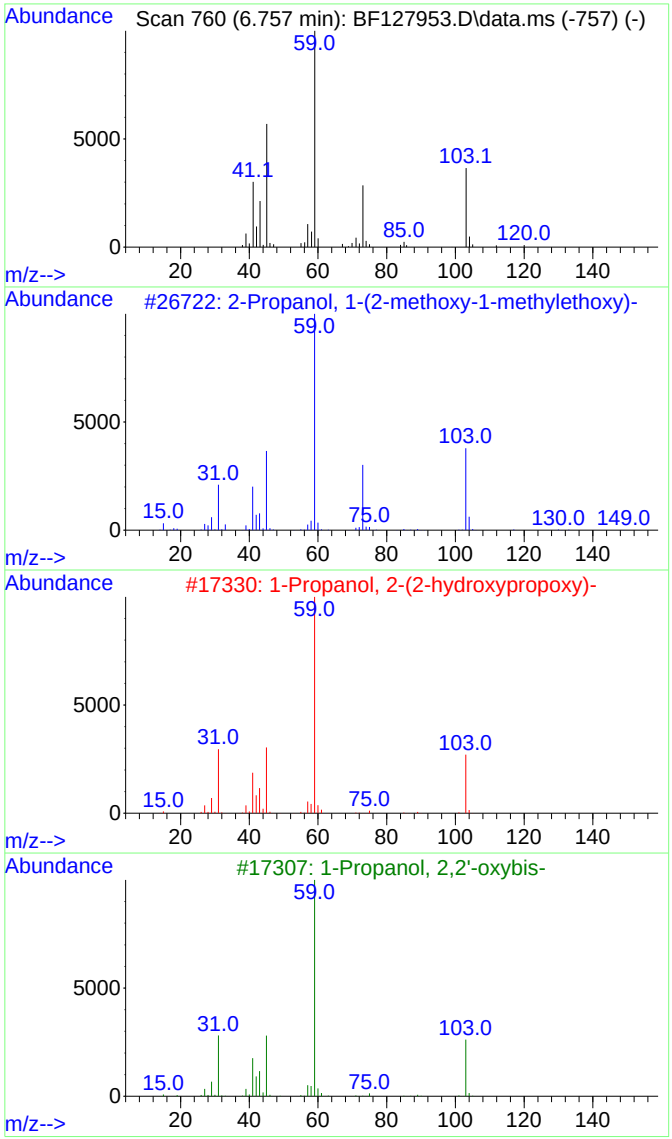
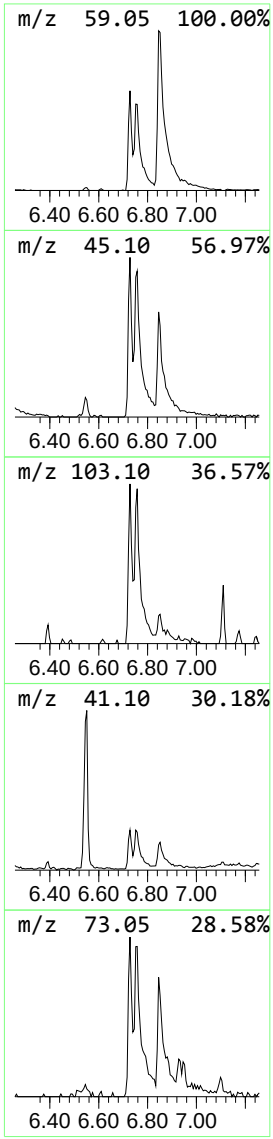
****
Peak Number 7 1-Propanol, 2-(2-hydroxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.757	5.30 ng	176199	1,4-Dichlorobenzene-d4	6.934

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	59
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59
4	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	50
5	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	45





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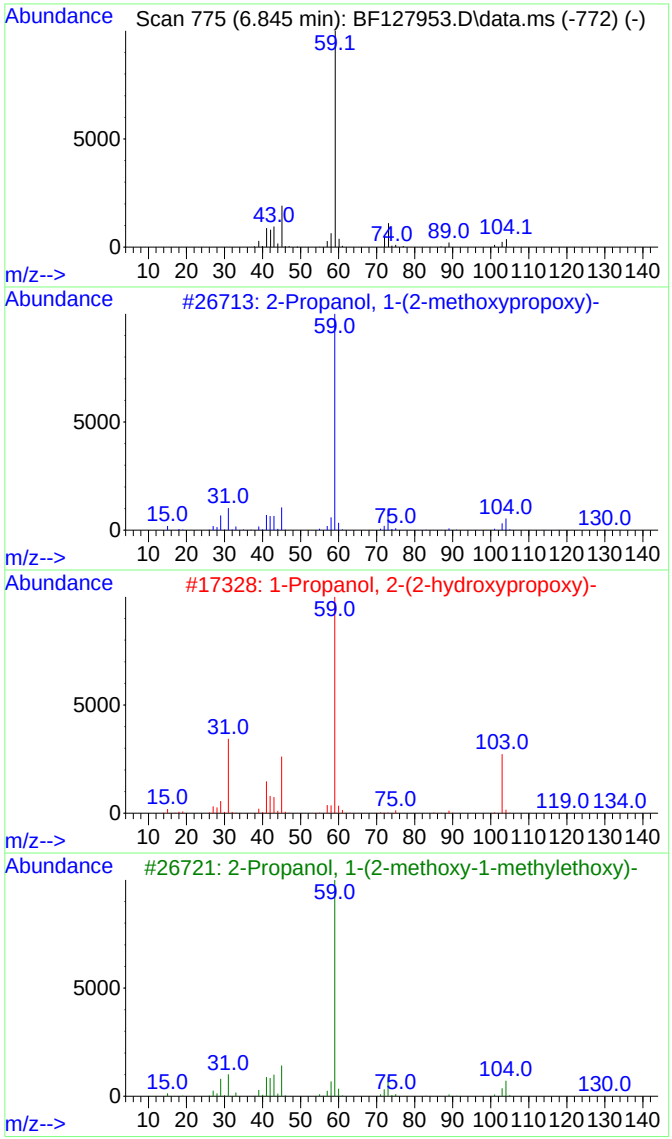
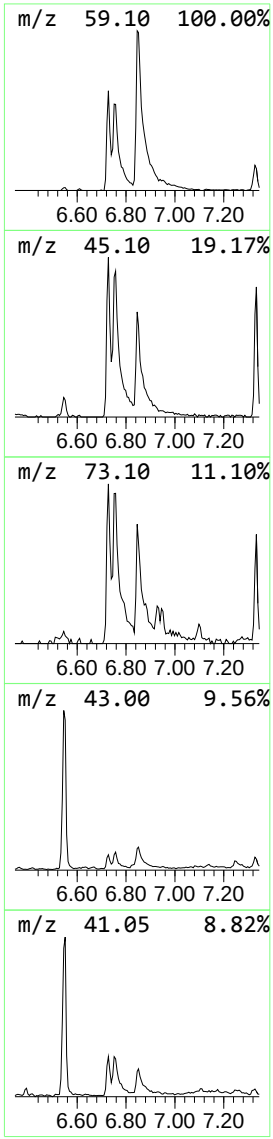
****
Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.845	7.12 ng	236605	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	72
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
3	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64





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TIC Library : C:\Database\NIST20.L
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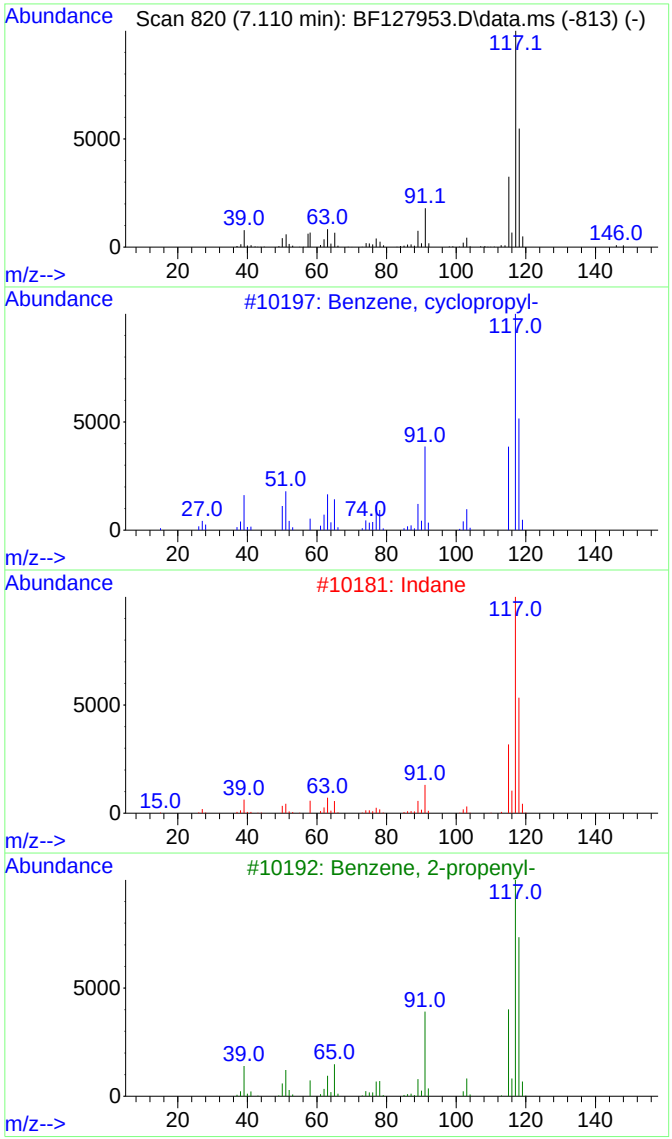
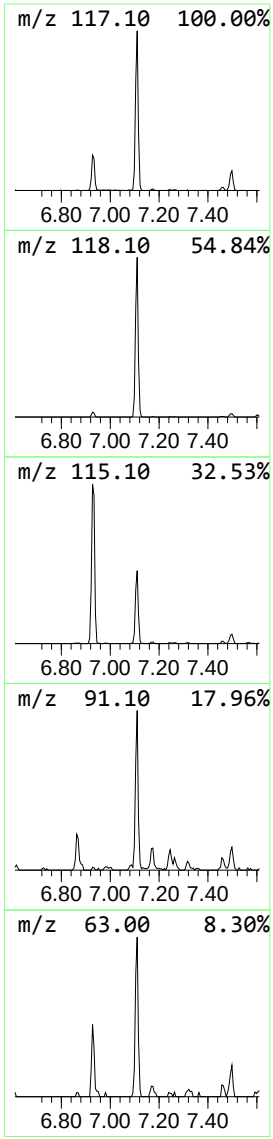
Peak Number 9 Benzene, cyclopropyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.110	8.64 ng	287291	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
2	Indane	118	C9H10	000496-11-7	91
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Deltacyclene	118	C9H10	007785-10-6	64
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53





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Data File : BF127953.D
Acq On : 27 Apr 2022 18:59
Operator : CG\JU
Sample : N2482-14
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-9

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

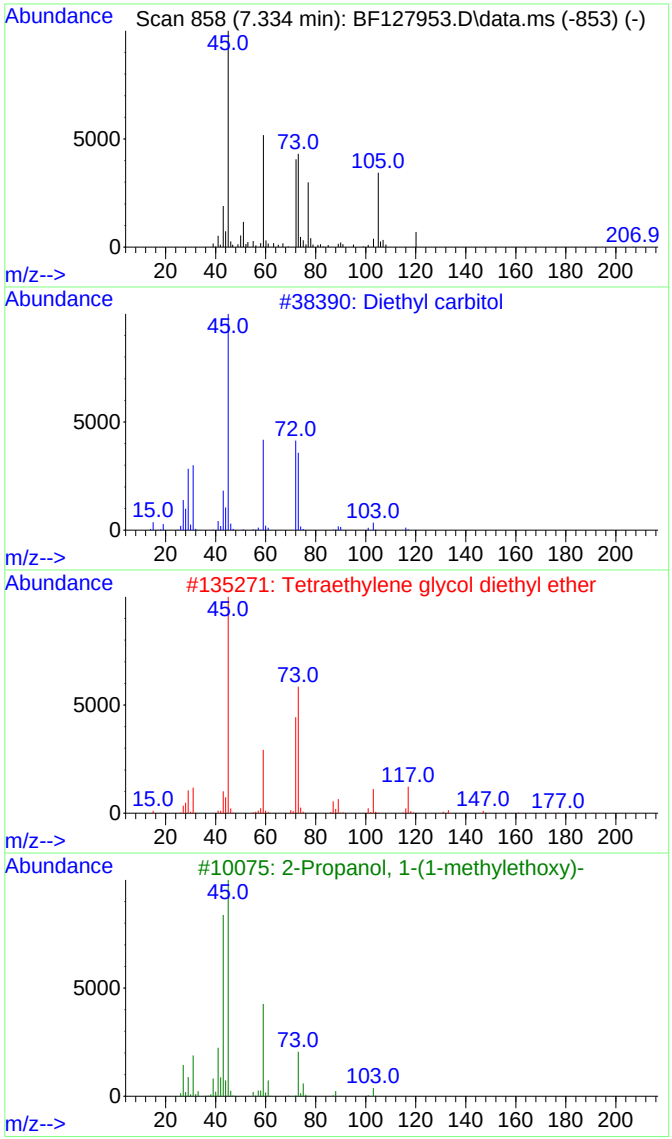
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

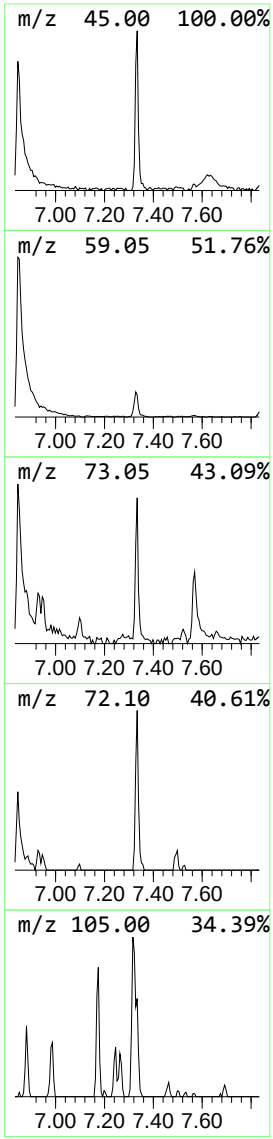
****

Peak Number 10 Diethyl carbitol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.334	2.93 ng	97448	1,4-Dichlorobenzene-d4	6.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl carbitol	162	C8H18O3	000112-36-7	53
2	Tetraethylene glycol diethyl ether	250	C12H26O5	004353-28-0	50
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	47
4	Ethyl 2-(2-(2-ethoxyethoxy)ethox...	220	C10H20O5	1000366-77-8	42
5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	40





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-9

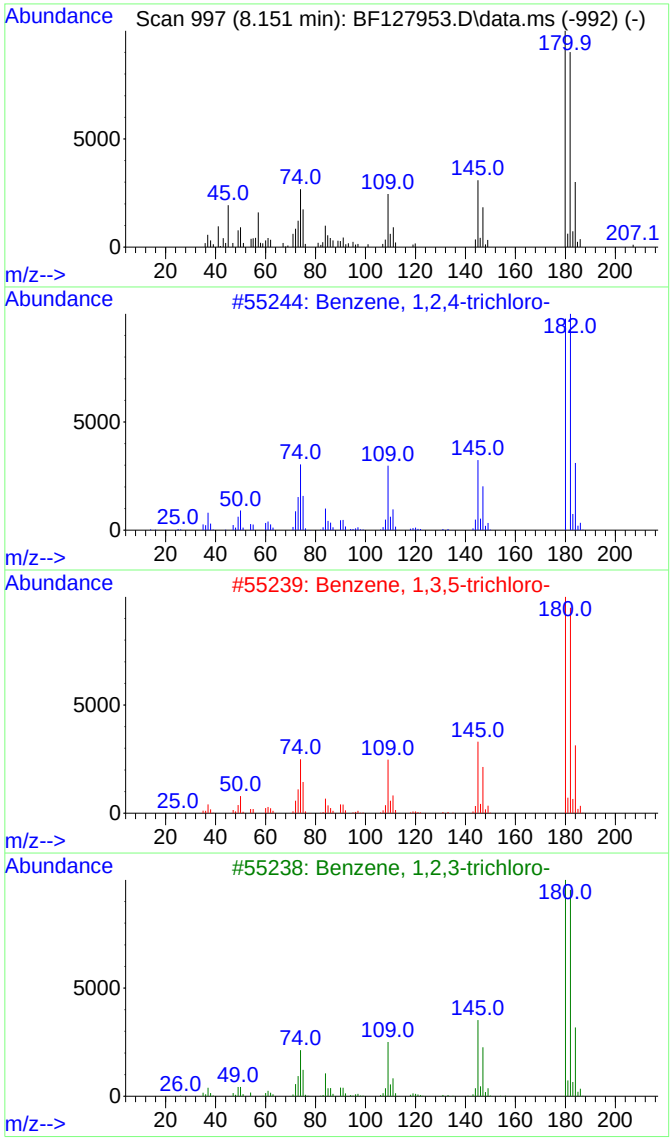
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

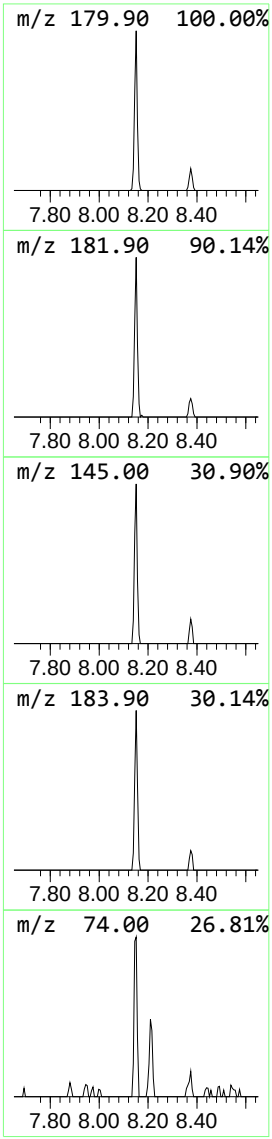
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, 1,2,4-trichloro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.151	2.48 ng	97406	Naphthalene-d8	8.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	98
2	Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
3	Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	96
4	4-Bromo-4-chloropyrazole	180	C3H2BrClN2	1000435-93-9	53
5	2,2-Dichloro-6-methyl-1-oxa-2-si...	180	C5H6Cl2OSi	067608-54-2	38





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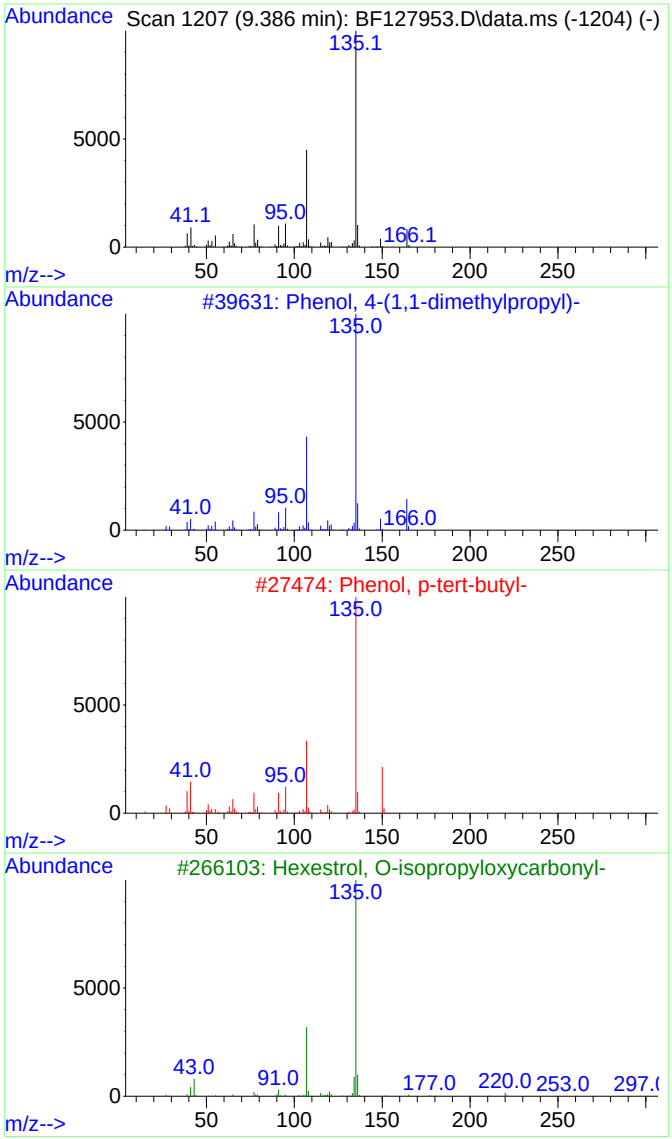
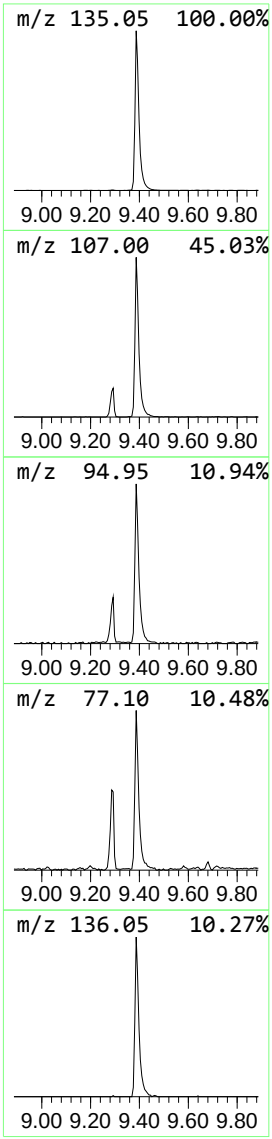
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.386	24.59 ng	1041790	Acenaphthene-d10	9.969

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-isopropyloxycarbonyl-	356	C22H28O4	1000487-68-4	64
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64





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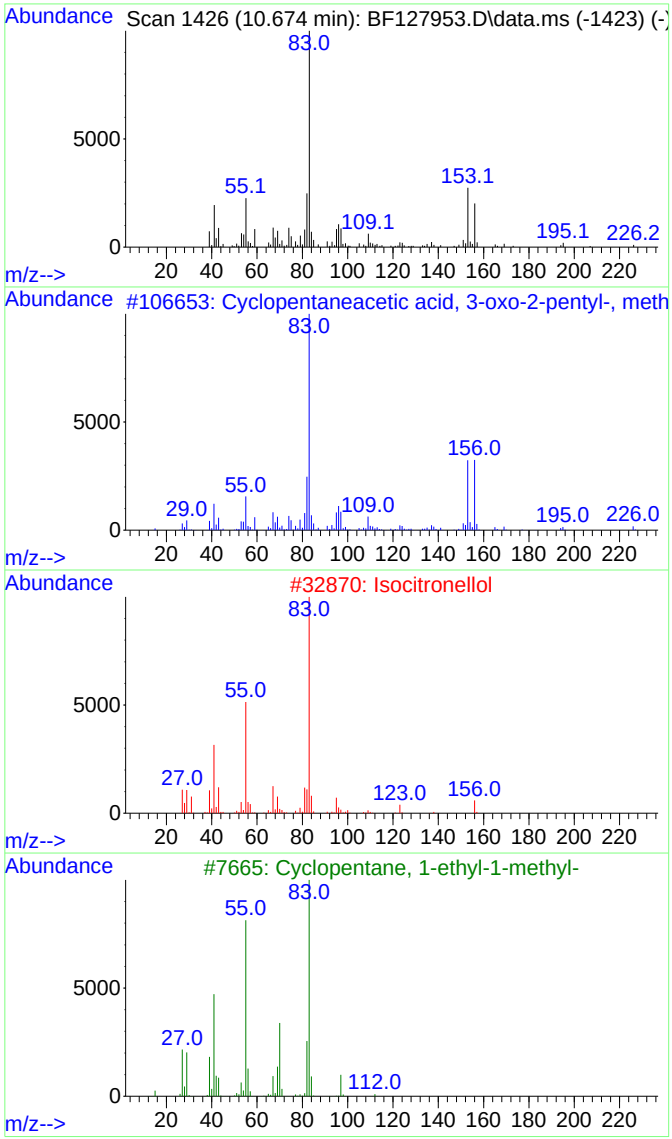
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

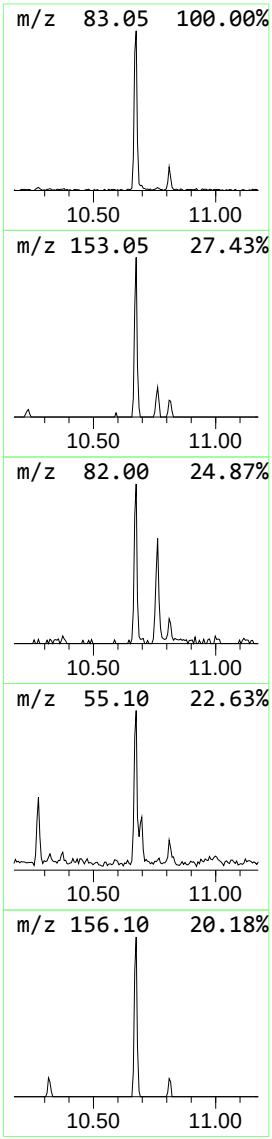
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Cyclopentaneacetic acid, 3-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	2.92 ng	123891	Acenaphthene-d10	9.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	97
2	Isocitronellol	156	C10H20O	018479-52-2	53
3	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	50
4	Heptadienyl tiglate, 2E, 4E-	194	C12H18O2	1000383-64-7	43
5	Cyclohexane, (2-nitro-2-propenyl)-	169	C9H15NO2	080255-17-0	43





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-9

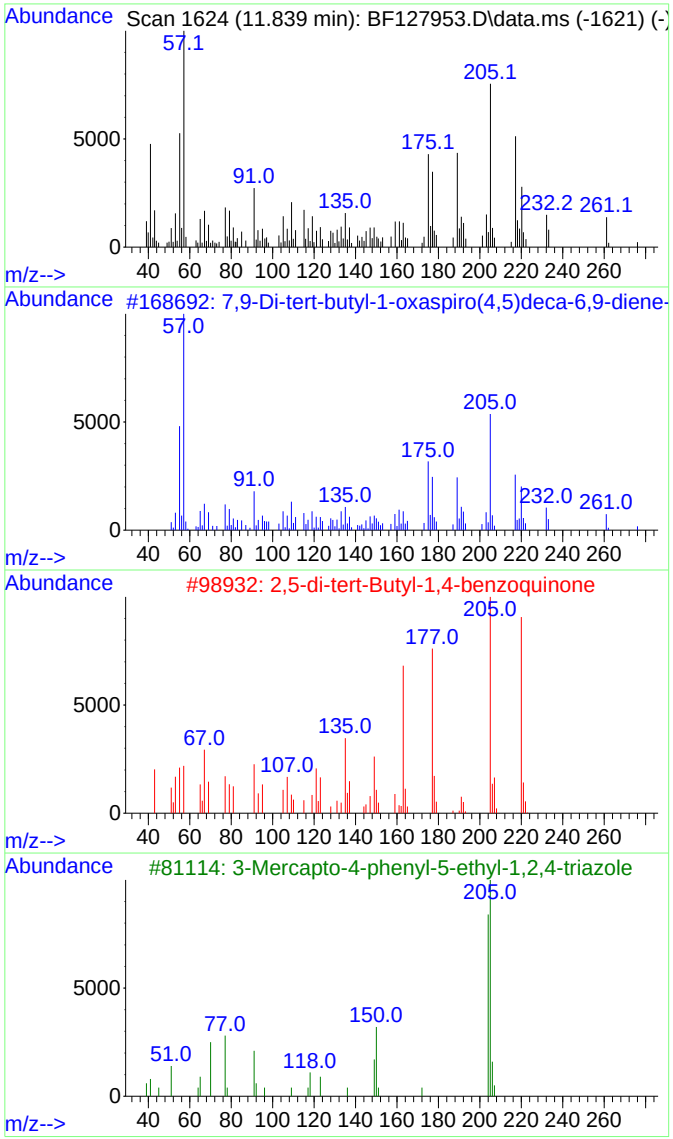
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

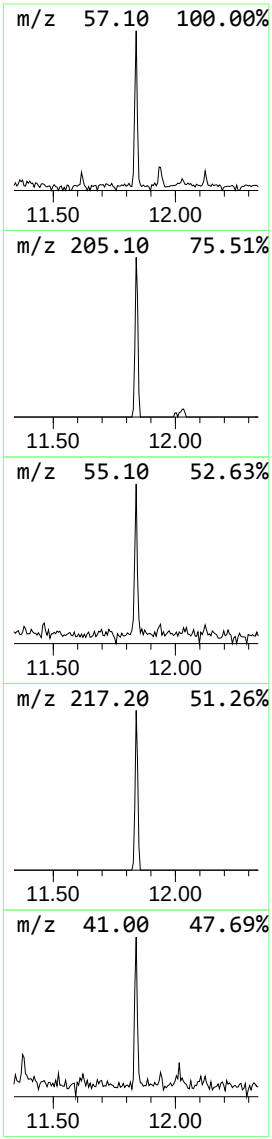
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.18 ng	76947	Phenanthrene-d10	11.463

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-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	53
3	3-Mercapto-4-phenyl-5-ethyl-1,2,...	205	C10H11N3S	029448-76-8	44
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38





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
Cyclopentanone	4.469	12.3	ng	409572	1	6.934	664682	20.0
Di-sec-Butyl ether	4.569	3.2	ng	107697	1	6.934	664682	20.0
unknown5.169	5.169	3.9	ng	130988	1	6.934	664682	20.0
Benzene, (1-met...	6.104	4.1	ng	137331	1	6.934	664682	20.0
Benzene, propyl-	6.392	4.3	ng	141603	1	6.934	664682	20.0
2-Propanol, 1-(...	6.728	3.2	ng	107192	1	6.934	664682	20.0
1-Propanol, 2-(...	6.757	5.3	ng	176199	1	6.934	664682	20.0
2-Propanol, 1-(...	6.845	7.1	ng	236605	1	6.934	664682	20.0
Benzene, cyclop...	7.110	8.6	ng	287291	1	6.934	664682	20.0
Diethyl carbitol	7.334	2.9	ng	97448	1	6.934	664682	20.0
Benzene, 1,2,4-...	8.151	2.5	ng	97406	2	8.210	785407	20.0
Phenol, 4-(1,1-...	9.386	24.6	ng	1041790	3	9.969	847347	20.0
Cyclopentaneace...	10.675	2.9	ng	123891	3	9.969	847347	20.0
7,9-Di-tert-but...	11.839	2.2	ng	76947	4	11.463	705832	20.0