

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
 Data File : BF127952.D
 Acq On : 27 Apr 2022 18:30
 Operator : CG\JU
 Sample : N2482-16
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SPN-7

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: BF127952.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.475	368	372	380	rVB	353808	421155	8.24%	1.552%
2	5.175	487	491	502	rBV	134070	166817	3.26%	0.615%
3	5.557	551	556	559	rBV	2816184	2716797	53.16%	10.011%
4	6.157	654	658	662	rBV	66146	53097	1.04%	0.196%
5	6.551	720	725	728	rBV	2256867	2228233	43.60%	8.211%
6	6.728	751	755	758	rBV	184938	193826	3.79%	0.714%
7	6.757	758	760	770	rVV	165546	236735	4.63%	0.872%
8	6.851	773	776	786	rVV	191333	313253	6.13%	1.154%
9	6.928	786	789	797	rVB	800377	719406	14.08%	2.651%
10	7.063	799	812	813	rBV4	19125	53332	1.04%	0.197%
11	7.104	813	819	825	rVV2	98231	127166	2.49%	0.469%
12	7.334	853	858	865	rVB3	48831	65838	1.29%	0.243%
13	7.498	880	886	889	rVB	2841329	3059484	59.86%	11.274%
14	7.945	956	962	965	rVB	53189	54731	1.07%	0.202%
15	8.151	993	997	999	rBV	81406	85161	1.67%	0.314%
16	8.210	1003	1007	1011	rBV	910834	853167	16.69%	3.144%
17	8.457	1037	1049	1052	rBV5	25599	79360	1.55%	0.292%
18	8.616	1073	1076	1086	rVB2	38249	52944	1.04%	0.195%
19	9.210	1170	1177	1178	rBV2	52635	73806	1.44%	0.272%
20	9.292	1185	1191	1194	rBV	5075017	5110757	100.00%	18.833%
21	9.386	1204	1207	1224	rVB	633590	812912	15.91%	2.996%
22	9.969	1301	1306	1310	rBV	1051316	935757	18.31%	3.448%
23	10.380	1372	1376	1380	rVB	182288	156736	3.07%	0.578%
24	10.675	1422	1426	1428	rBV	165682	138292	2.71%	0.510%
25	10.763	1436	1441	1445	rBV	2825161	2671042	52.26%	9.843%
26	11.463	1556	1560	1563	rBV	1015053	842835	16.49%	3.106%
27	11.839	1621	1624	1627	rBV	101132	74627	1.46%	0.275%
28	13.051	1825	1830	1833	rBV	3838976	3633986	71.10%	13.391%
29	14.104	2006	2009	2017	rVB	548857	538678	10.54%	1.985%
30	15.615	2261	2266	2277	rBV	484014	667651	13.06%	2.460%

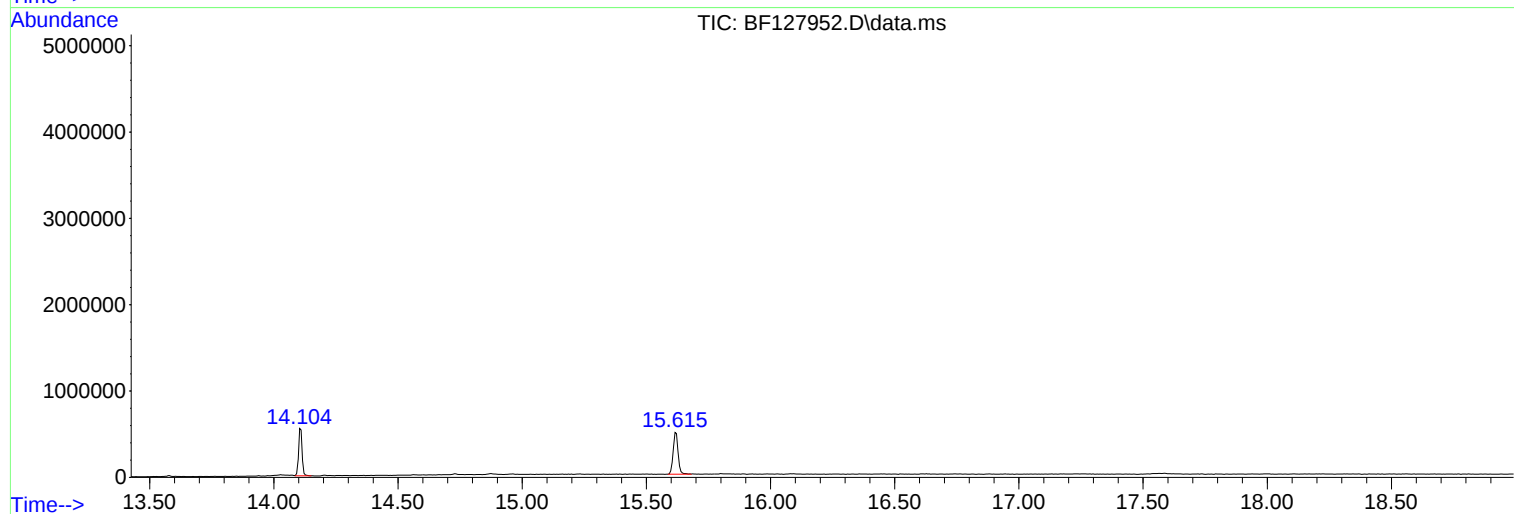
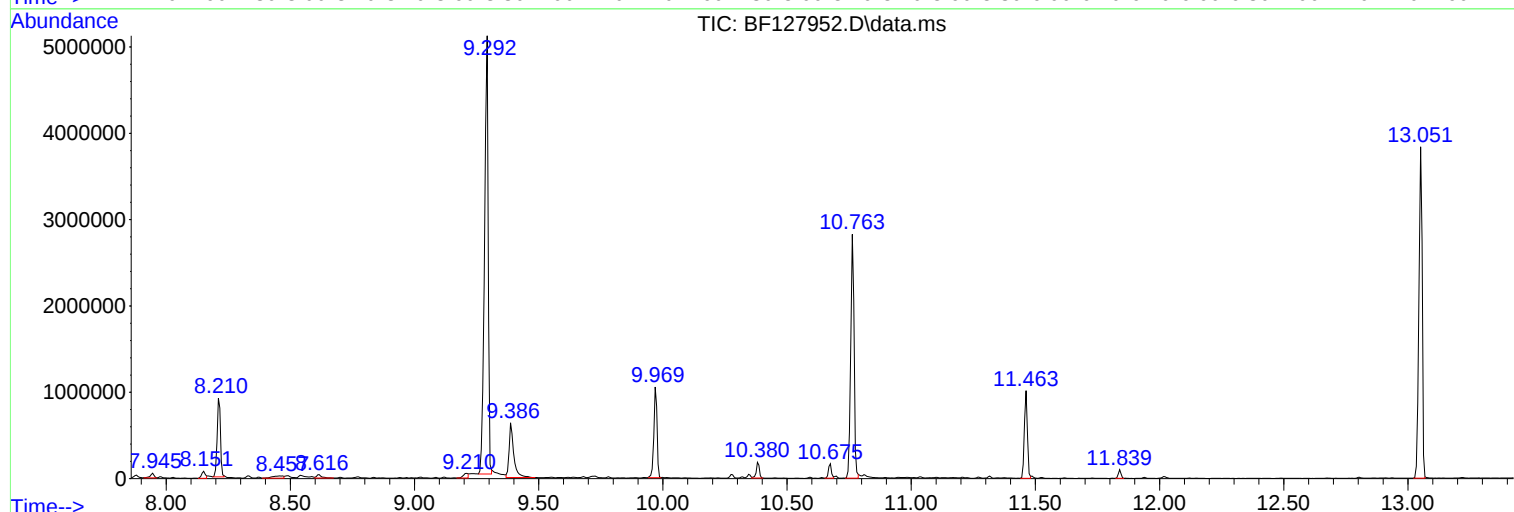
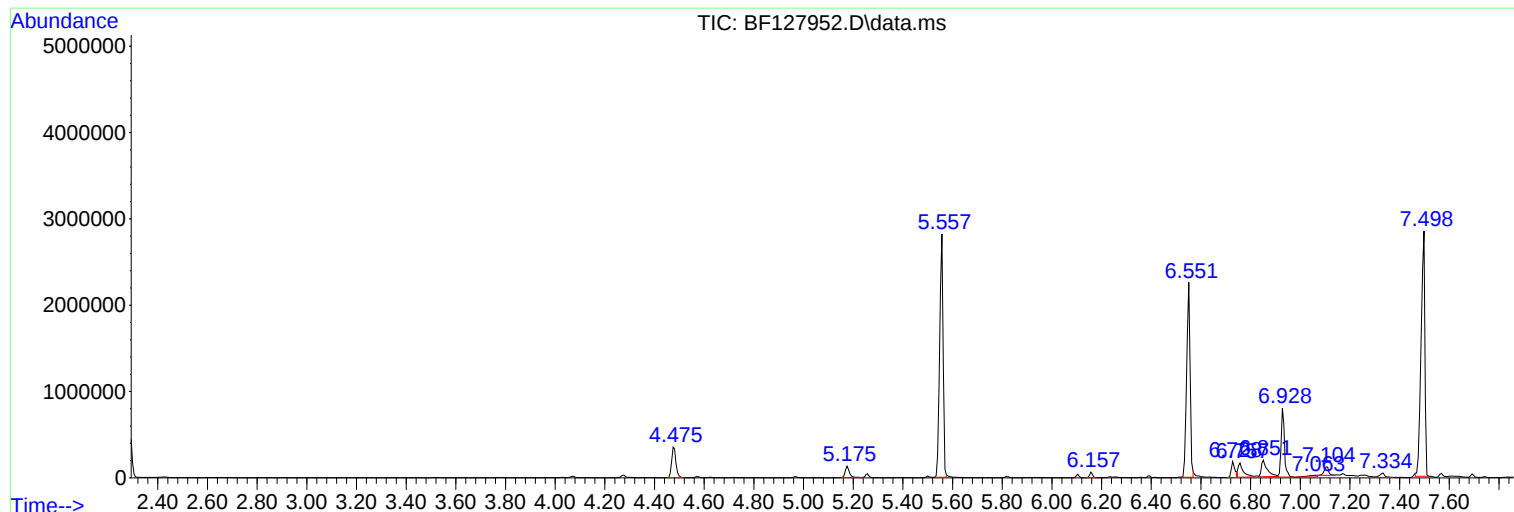
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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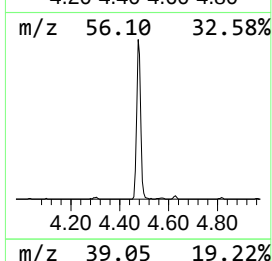
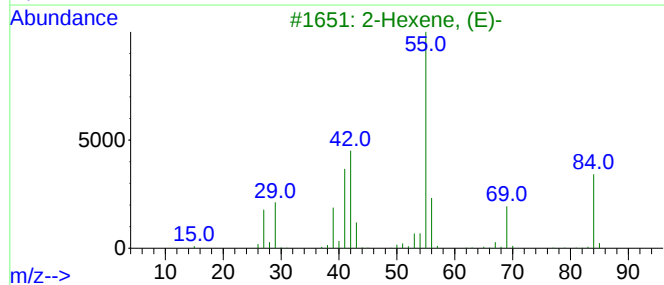
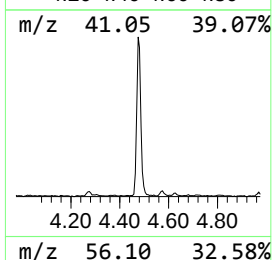
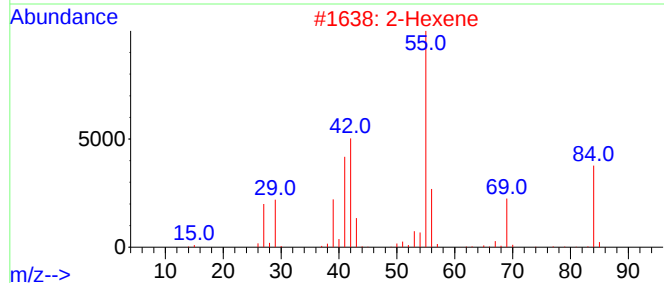
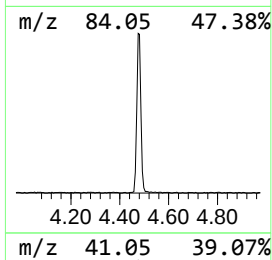
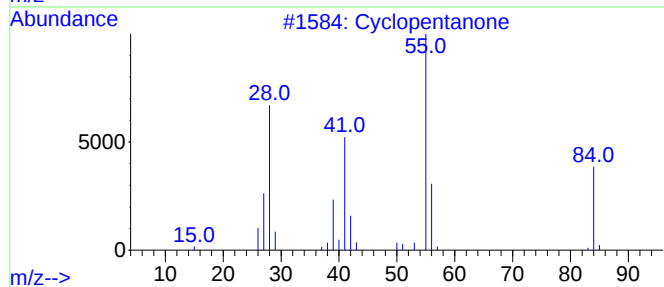
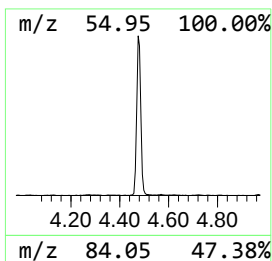
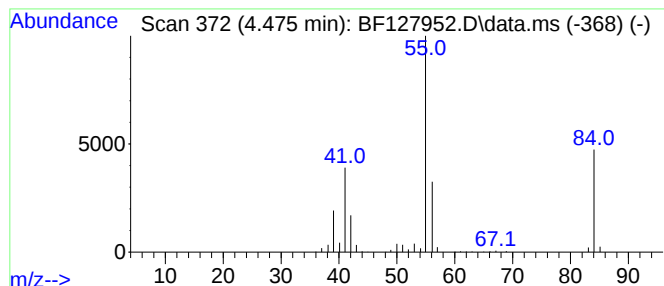
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	11.71 ng	421155	1,4-Dichlorobenzene-d4	6.928

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentanone	84	C5H8O	000120-92-3	90
2		2-Hexene	84	C6H12	000592-43-8	64
3		2-Hexene, (E)-	84	C6H12	004050-45-7	64
4		3-Hexene	84	C6H12	000592-47-2	50
5		3-Hexene, (Z)-	84	C6H12	007642-09-3	50



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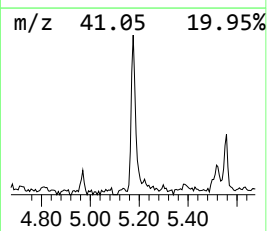
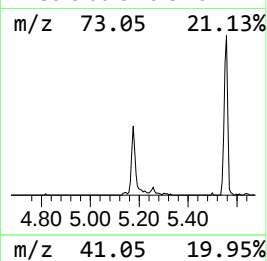
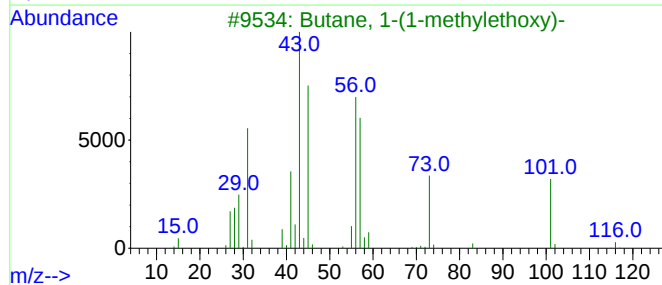
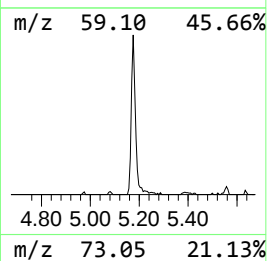
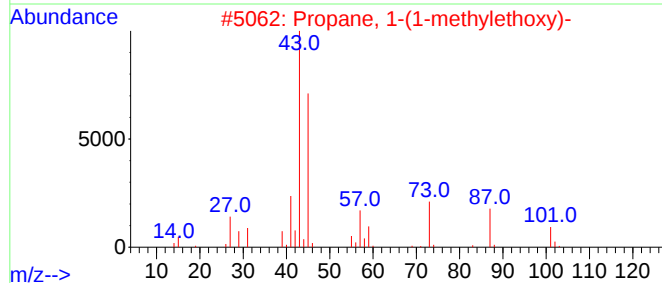
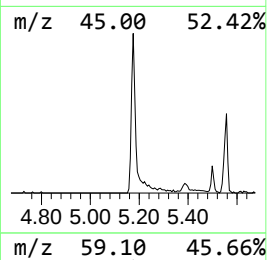
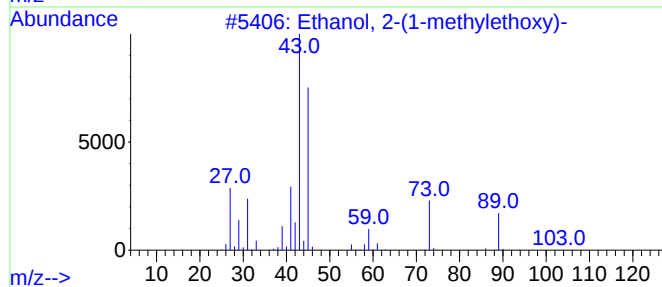
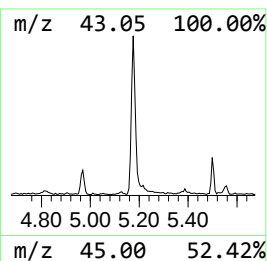
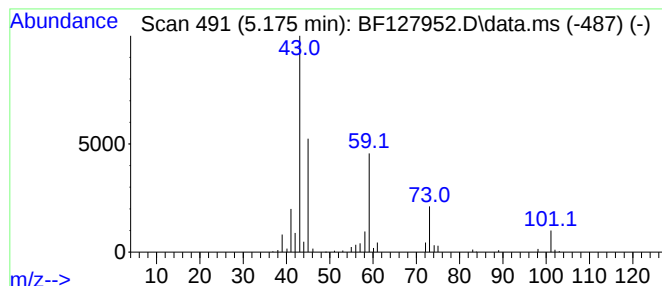
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.175 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	4.64 ng	166817	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	43
2			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	40
3			Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	40
4			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	38
5			Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	37



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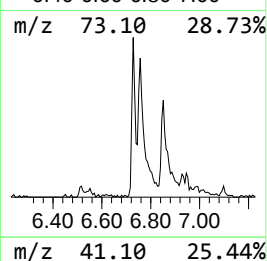
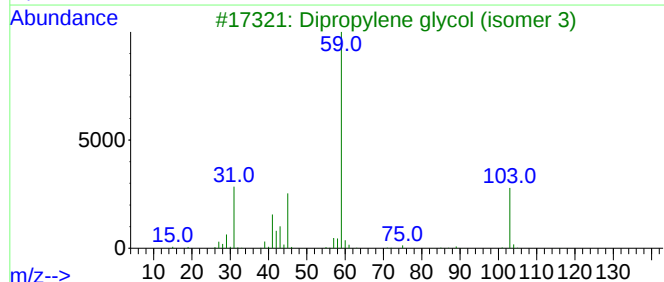
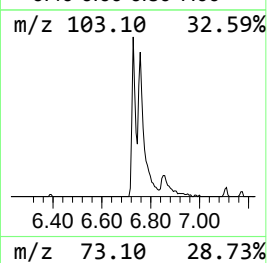
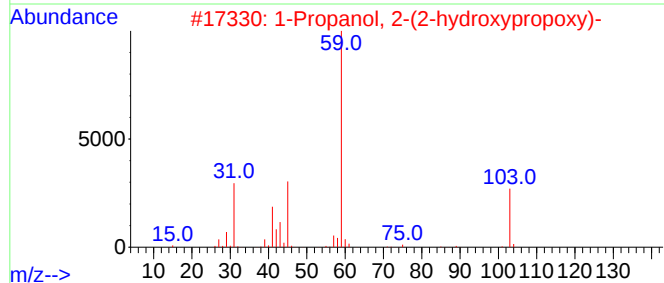
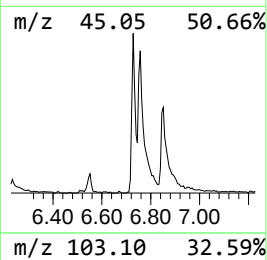
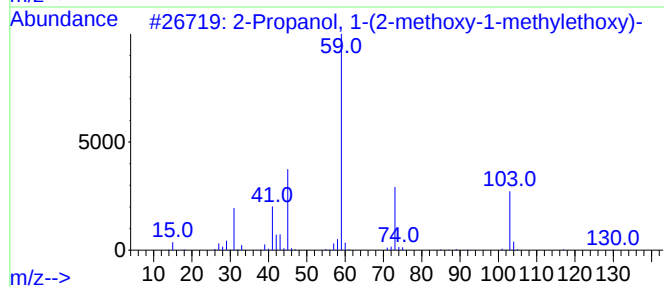
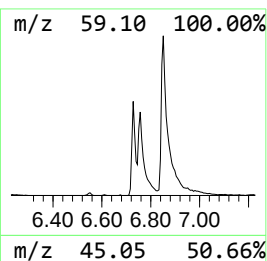
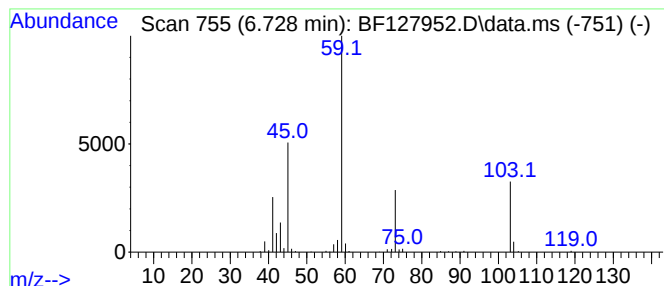
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	5.39 ng	193826	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	50
4			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42
5			Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	40



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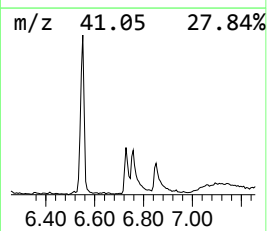
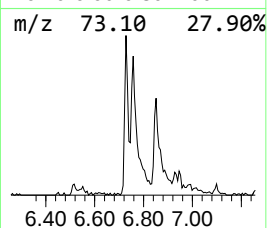
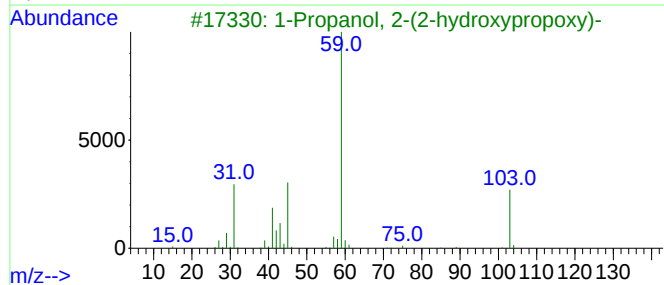
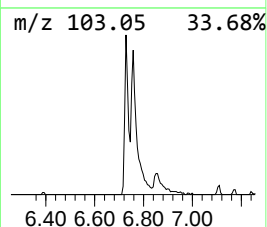
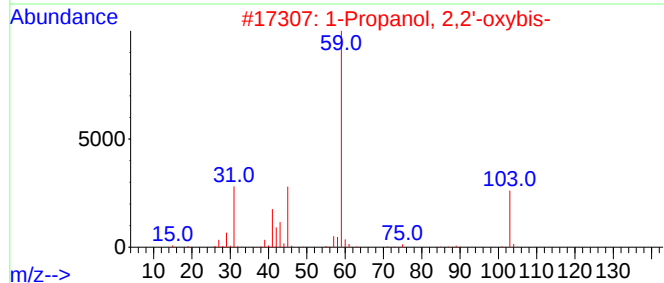
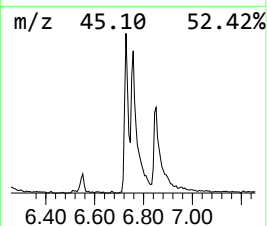
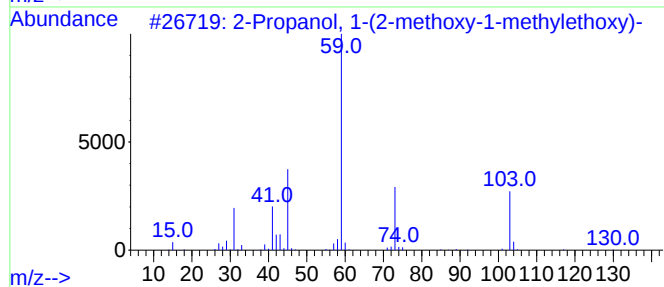
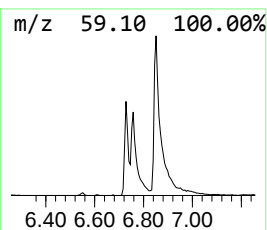
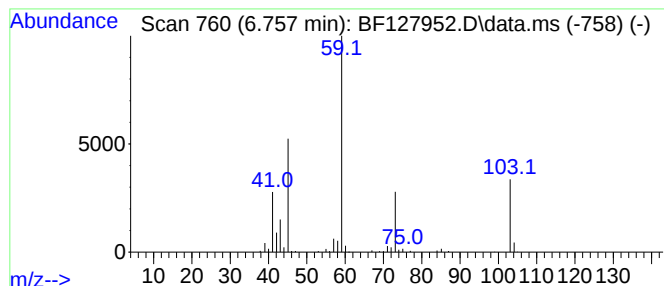
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Peak Number 4 1-Propanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.757	6.58 ng	236735	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53		
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53		



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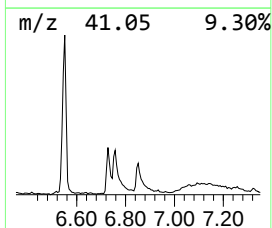
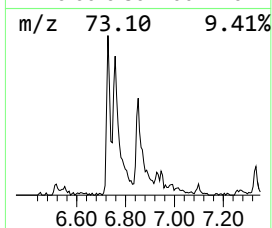
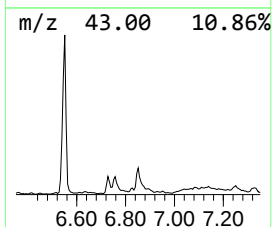
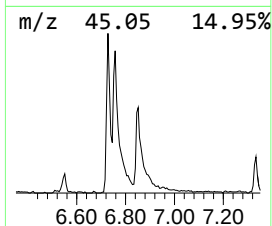
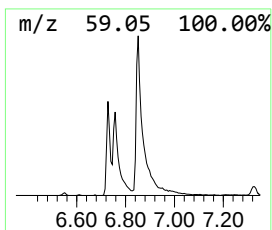
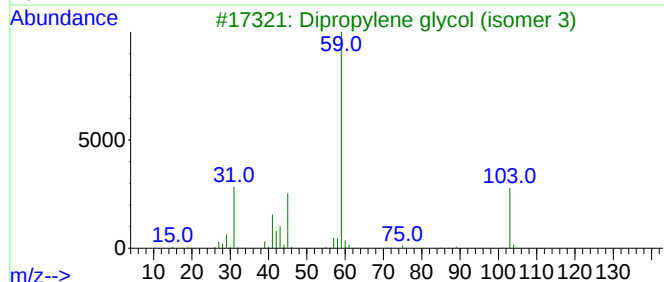
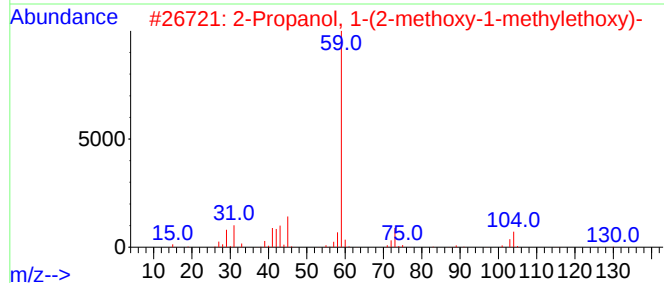
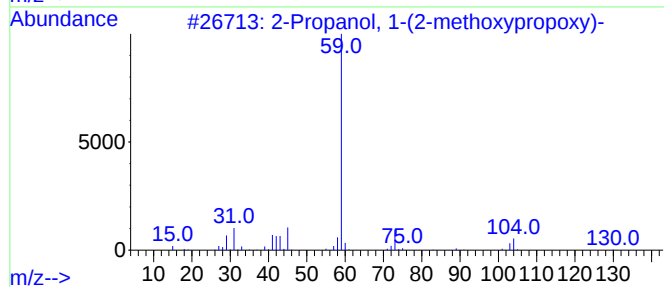
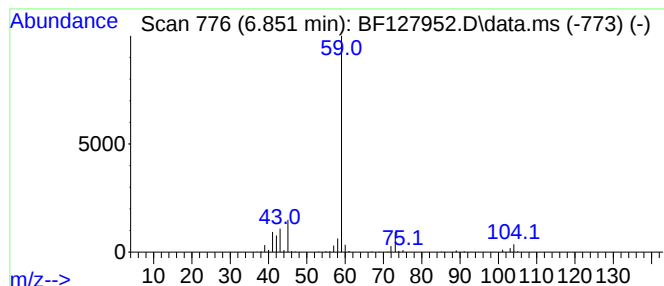
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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.851	8.71 ng	313253	1,4-Dichlorobenzene-d4	6.928

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	83
3			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64
4			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5			2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	50



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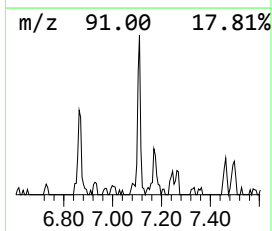
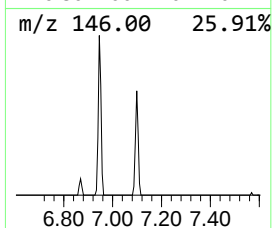
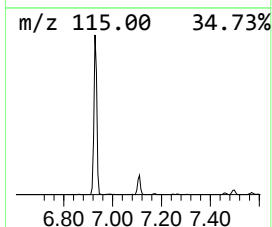
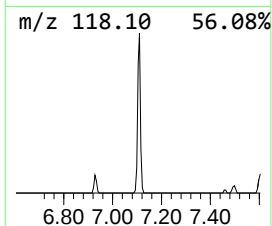
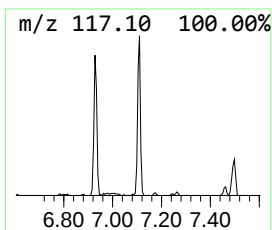
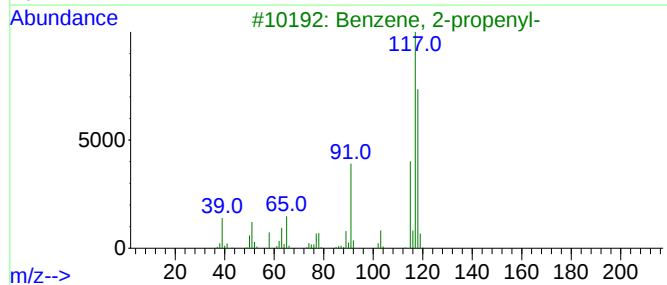
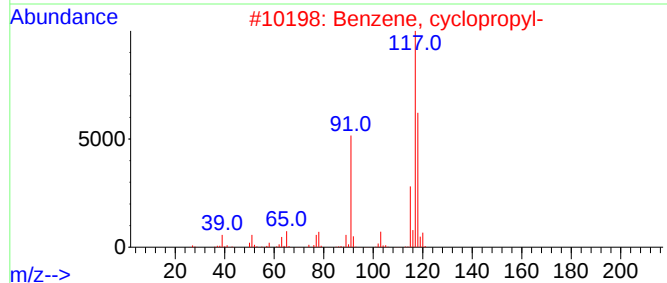
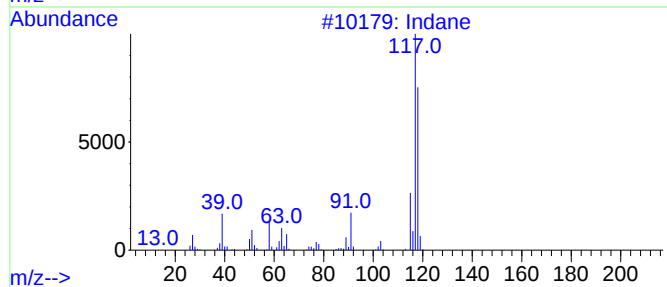
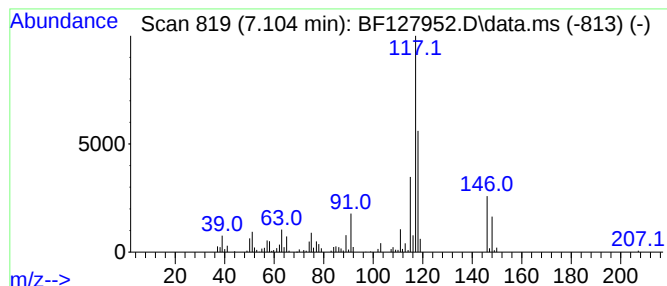
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Indane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.104	3.54 ng	127166	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	83
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	60
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
Data File : BF127952.D
Acq On : 27 Apr 2022 18:30
Operator : CG\JU
Sample : N2482-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-7

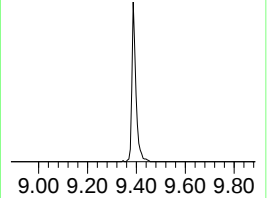
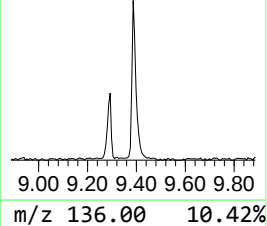
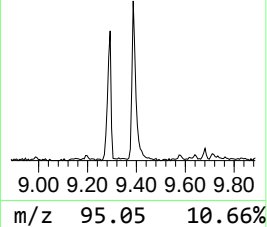
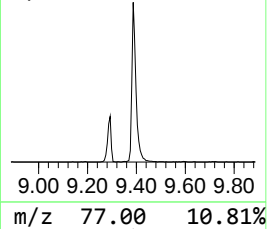
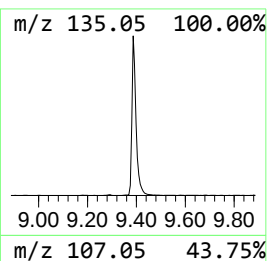
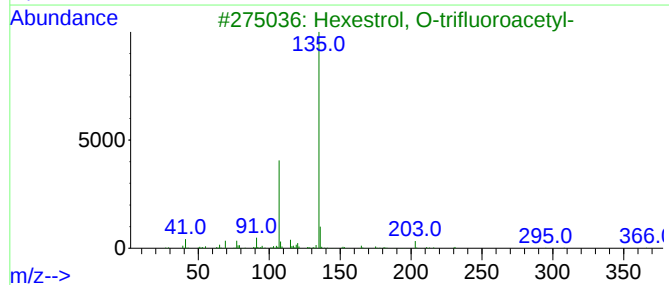
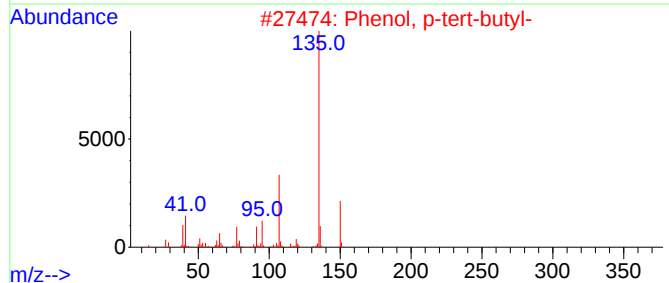
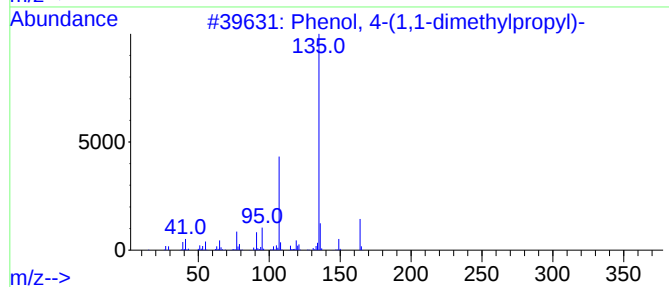
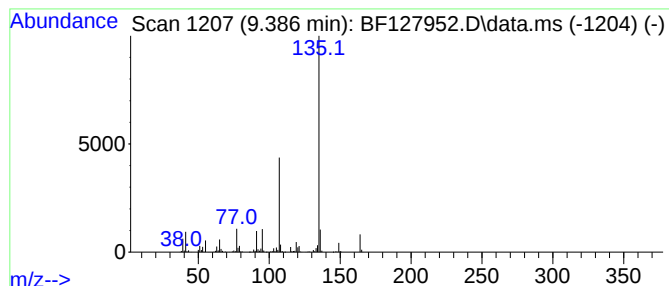
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.386	17.37 ng	812912	Acenaphthene-d10	9.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
3			Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
4			4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
Data File : BF127952.D
Acq On : 27 Apr 2022 18:30
Operator : CG\JU
Sample : N2482-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-7

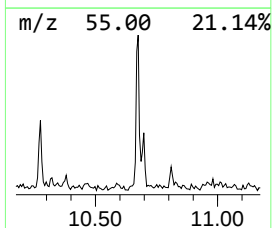
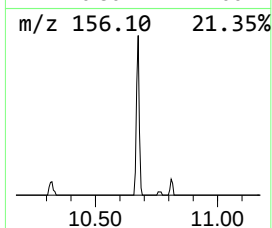
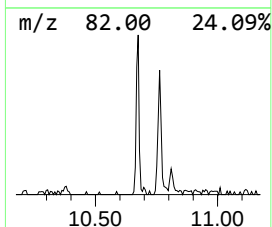
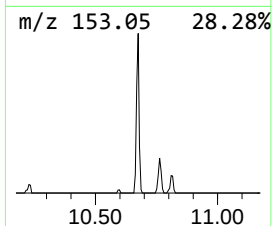
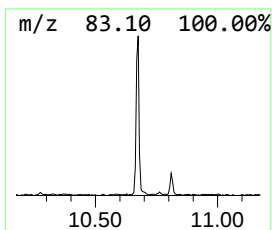
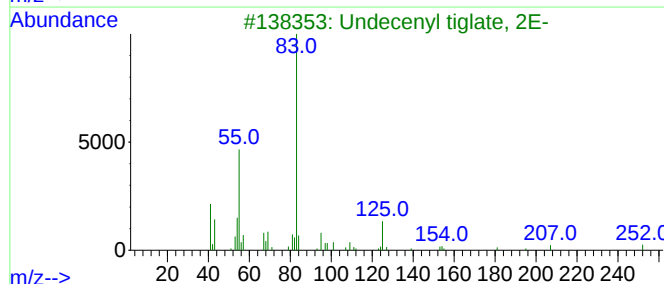
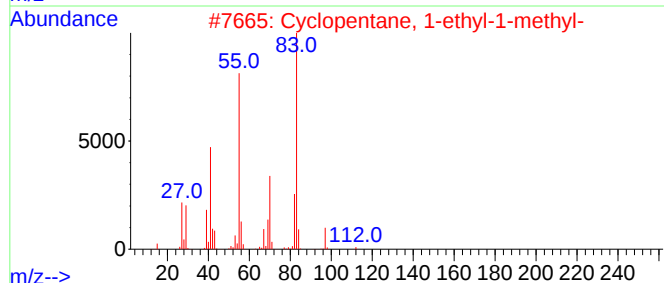
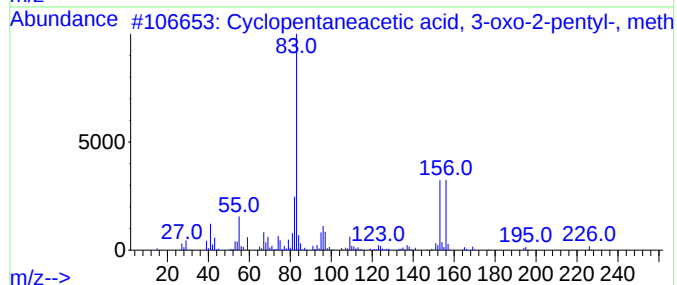
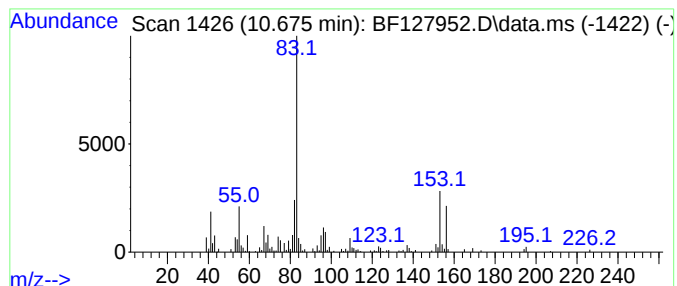
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentaneacetic acid, 3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	2.96 ng	138292	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			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47
3			Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	43
4			Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	38
5			Prop-2-ynyl (E)-2-methylbut-2-en...	138	C8H10O2	1000373-72-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042722\
Data File : BF127952.D
Acq On : 27 Apr 2022 18:30
Operator : CG\JU
Sample : N2482-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SPN-7

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentanone	4.475	11.7	ng	421155	1	6.928	719406	20.0
unknown5.175	5.175	4.6	ng	166817	1	6.928	719406	20.0
2-Propanol, 1-(...	6.728	5.4	ng	193826	1	6.928	719406	20.0
1-Propanol, 2,2...	6.757	6.6	ng	236735	1	6.928	719406	20.0
2-Propanol, 1-(...	6.851	8.7	ng	313253	1	6.928	719406	20.0
Indane	7.104	3.5	ng	127166	1	6.928	719406	20.0
Phenol, 4-(1,1-...	9.386	17.4	ng	812912	3	9.969	935757	20.0
Cyclopentaneace...	10.675	3.0	ng	138292	3	9.969	935757	20.0