

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
 Data File : BF130940.D
 Acq On : 02 Nov 2022 20:35
 Operator : CG\JU
 Sample : N5395-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-2-103122

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130940.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	31	rVB	385874	501154	28.58%	3.763%
2	2.340	39	43	50	rVB	33953	42542	2.43%	0.319%
3	4.034	326	331	338	rVB	113190	139311	7.94%	1.046%
4	5.151	516	521	534	rVB	361558	420800	24.00%	3.159%
5	5.540	582	587	590	rBV	1699581	1661325	94.74%	12.474%
6	6.545	752	758	761	rBV	1670121	1695521	96.69%	12.730%
7	6.922	818	822	826	rBV	545681	422688	24.10%	3.174%
8	7.316	885	889	899	rVB	52501	54909	3.13%	0.412%
9	7.486	913	918	921	rBV	1247494	1080975	61.64%	8.116%
10	8.104	1020	1023	1035	rBV	125371	241683	13.78%	1.815%
11	8.210	1037	1041	1043	rVV	588004	538128	30.69%	4.040%
12	8.228	1043	1044	1047	rVB	38897	23265	1.33%	0.175%
13	9.286	1219	1224	1227	rBV	2148051	1753617	100.00%	13.167%
14	9.969	1336	1340	1343	rVB	653931	516433	29.45%	3.878%
15	10.610	1446	1449	1455	rVB2	26427	25196	1.44%	0.189%
16	10.757	1470	1474	1477	rBV	1131074	904702	51.59%	6.793%
17	10.804	1479	1482	1485	rVB	45262	36349	2.07%	0.273%
18	10.880	1490	1495	1498	rBV	21664	27304	1.56%	0.205%
19	11.345	1571	1574	1580	rVB4	17095	22675	1.29%	0.170%
20	11.457	1590	1593	1596	rBV	486525	433122	24.70%	3.252%
21	11.480	1596	1597	1600	rVB	78451	53829	3.07%	0.404%
22	11.845	1656	1659	1662	rBV	54642	37842	2.16%	0.284%
23	11.974	1676	1681	1682	rBV2	24389	29112	1.66%	0.219%
24	12.074	1694	1698	1701	rBV3	16913	21049	1.20%	0.158%
25	12.557	1775	1780	1785	rBV3	47002	51663	2.95%	0.388%
26	12.674	1797	1800	1803	rBV	120289	99306	5.66%	0.746%
27	12.910	1834	1840	1843	rBV	94554	109875	6.27%	0.825%
28	13.051	1860	1864	1867	rVB	1286935	1098823	62.66%	8.250%
29	13.186	1884	1887	1890	rBV	32106	30700	1.75%	0.231%
30	13.233	1893	1895	1898	rVB	23010	22398	1.28%	0.168%
31	14.027	2025	2030	2031	rBV5	28124	44245	2.52%	0.332%
32	14.110	2039	2044	2046	rBV2	396773	399316	22.77%	2.998%
33	14.133	2046	2048	2051	rVB	55980	41098	2.34%	0.309%
34	14.568	2120	2122	2125	rVB	26429	25418	1.45%	0.191%
35	15.174	2221	2225	2228	rBV	50004	81696	4.66%	0.613%
36	15.245	2234	2237	2241	rVB	46452	50083	2.86%	0.376%

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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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.551	2286	2289	2293	rBV	40908	43946	2.51%	0.330%
38	15.621	2296	2301	2310	rBV	332357	443977	25.32%	3.334%
39	15.857	2339	2341	2345	rVB5	29022	36207	2.06%	0.272%
40	16.109	2381	2384	2390	rVB2	38172	56352	3.21%	0.423%

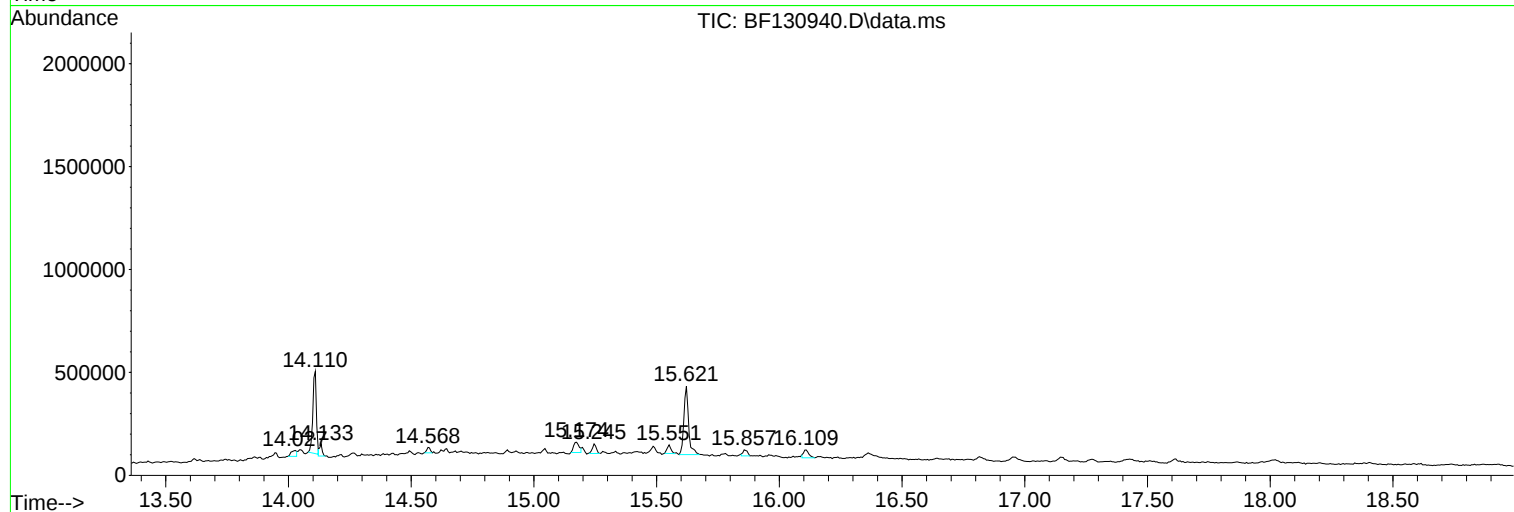
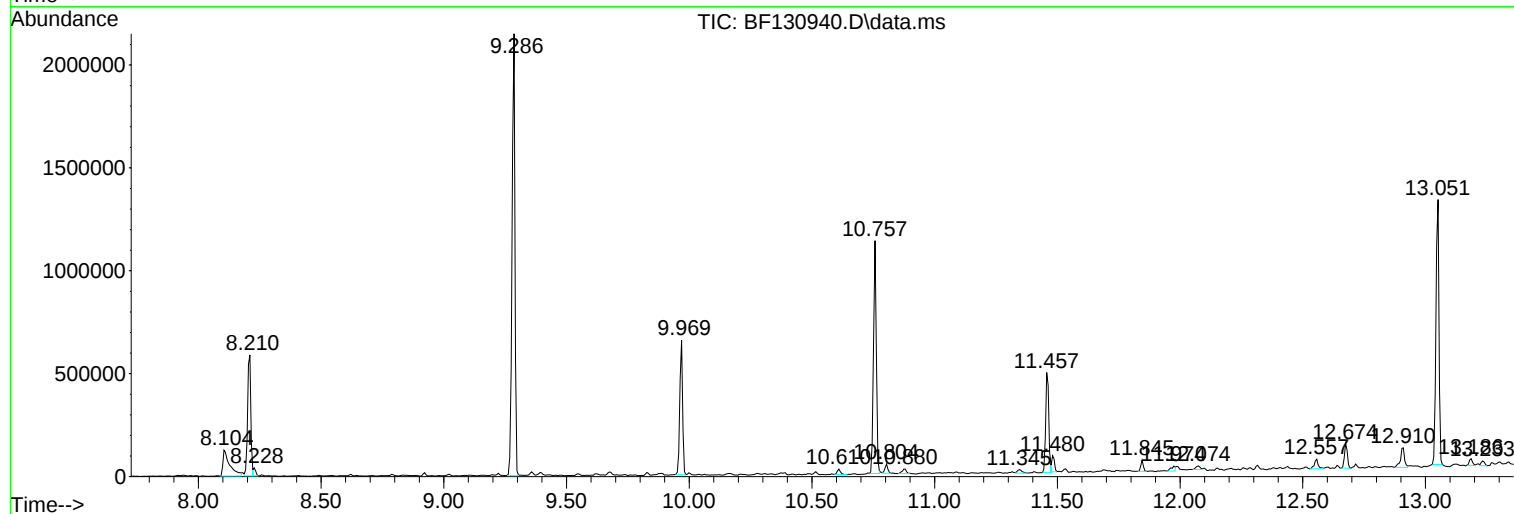
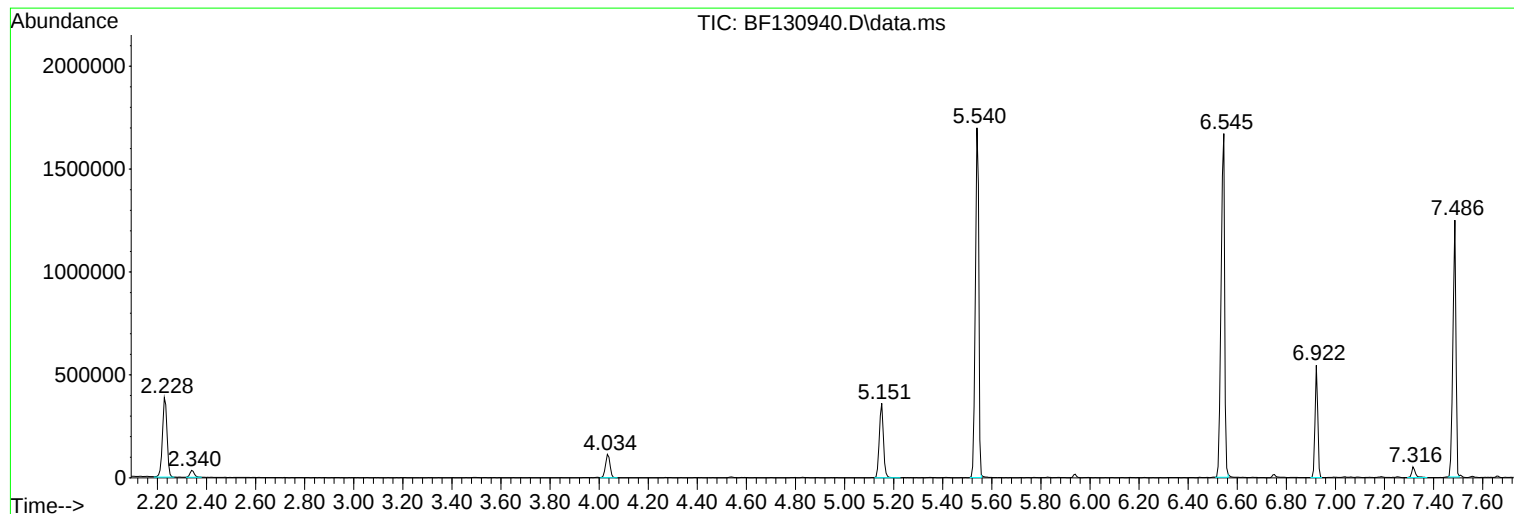
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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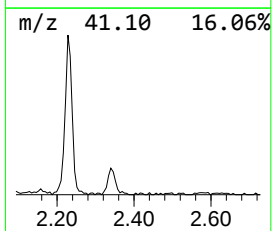
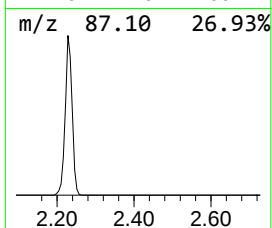
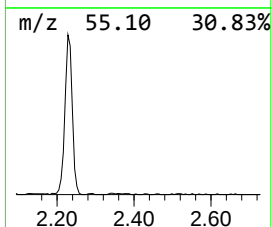
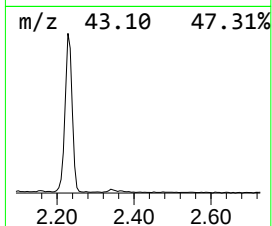
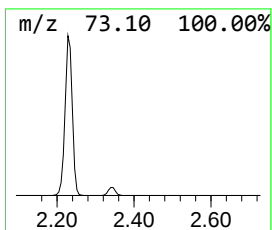
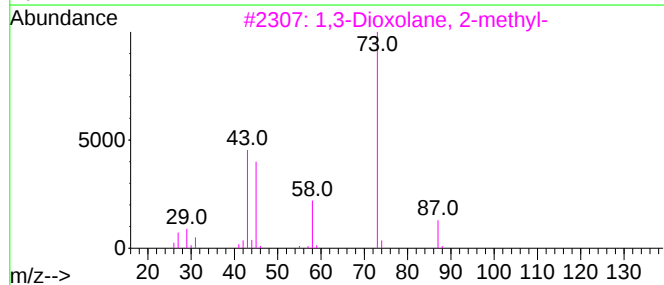
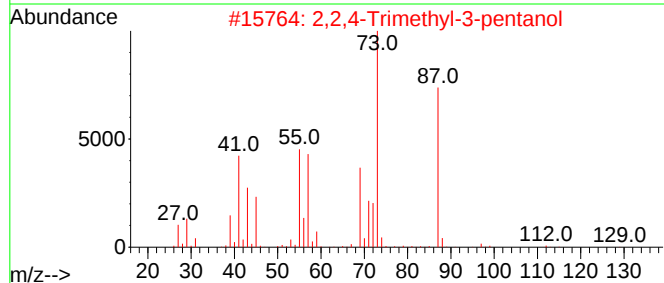
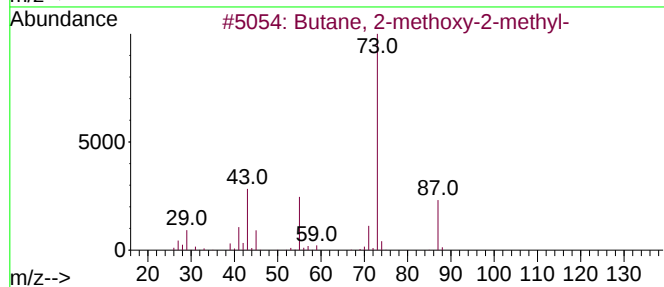
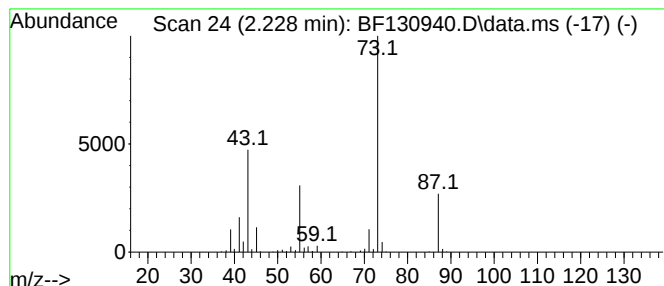
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	23.71 ng	501154	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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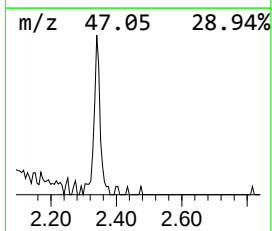
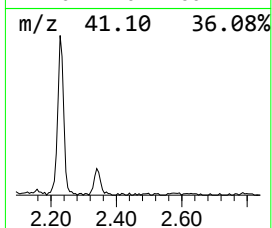
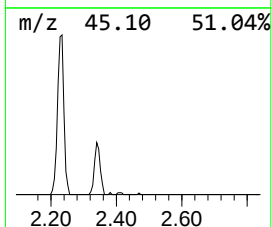
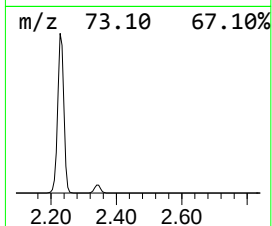
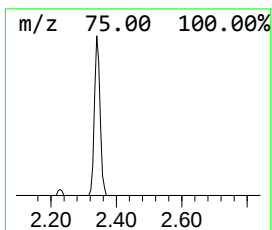
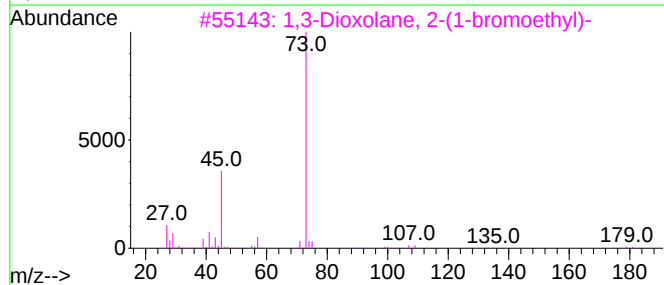
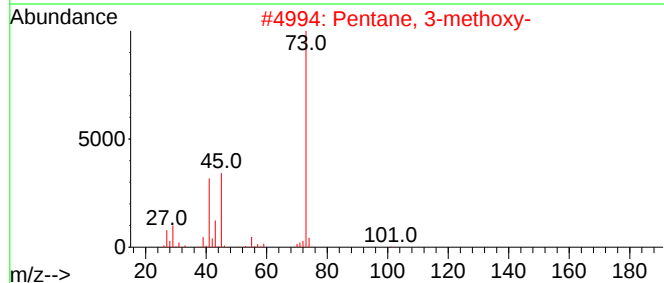
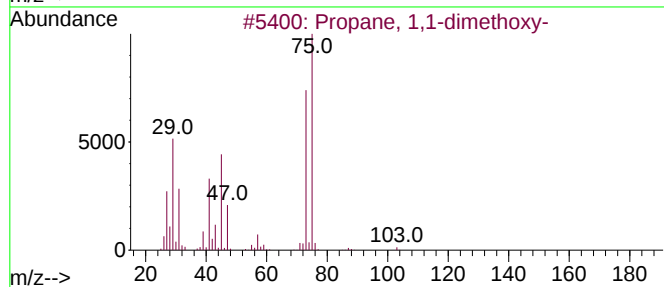
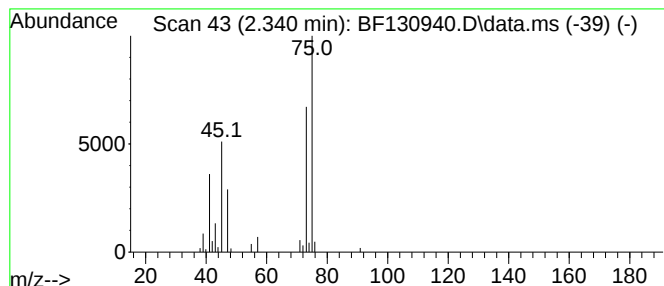
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	2.01 ng	42542	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
5			Formamide, N-methylthio	75	C2H5NS	018952-41-5	7



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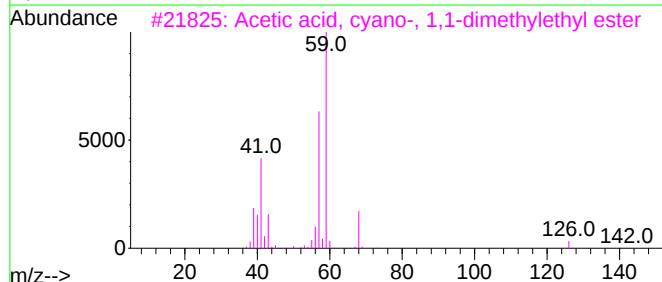
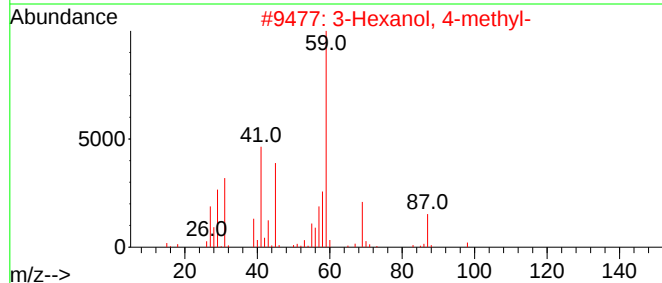
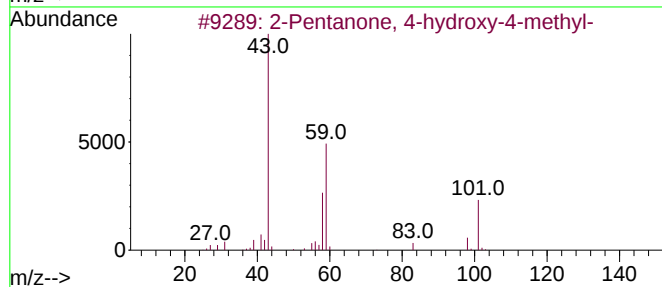
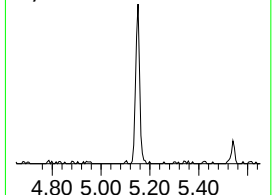
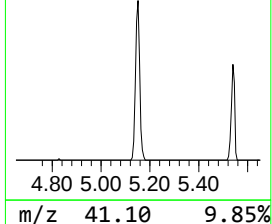
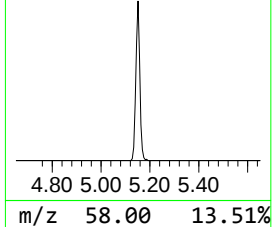
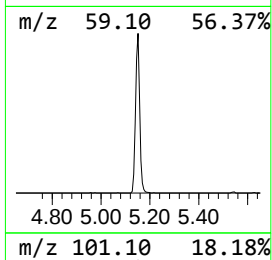
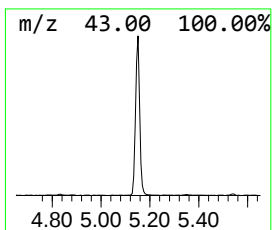
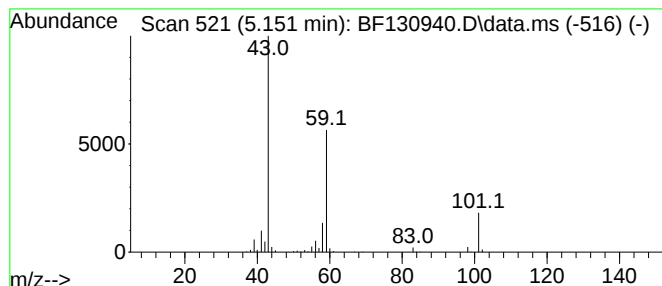
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	19.91 ng	420800	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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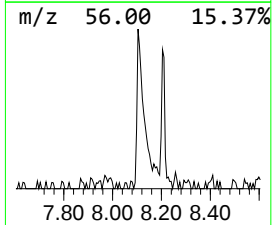
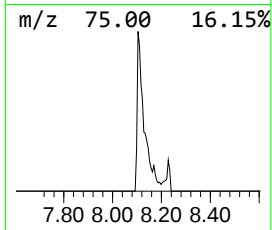
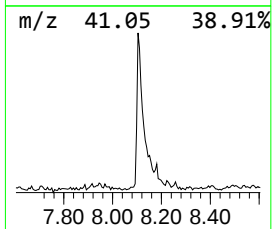
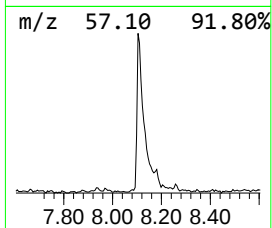
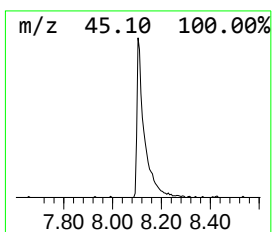
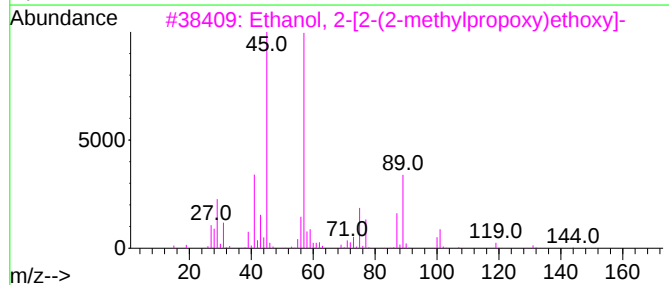
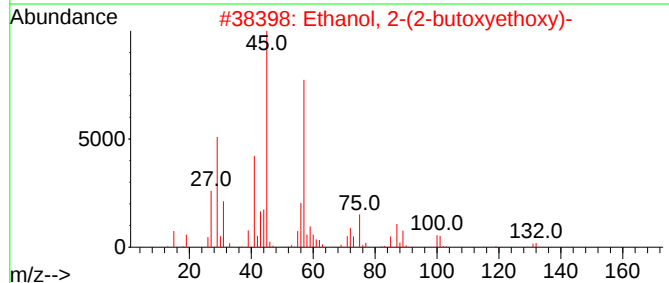
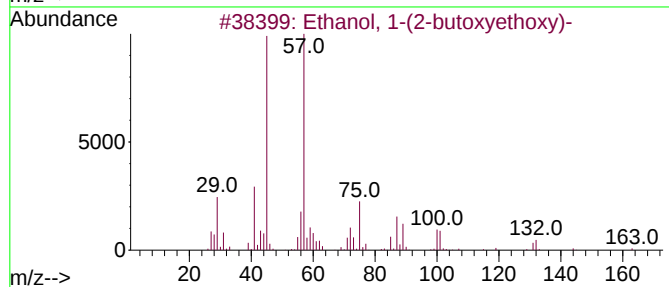
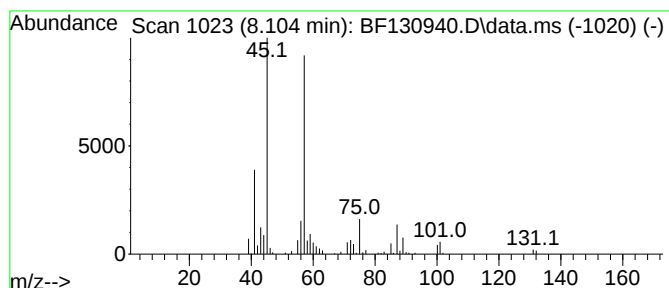
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	8.98 ng	241683	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	53



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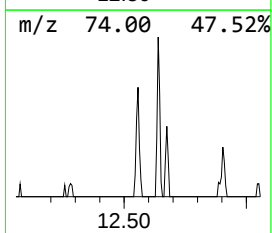
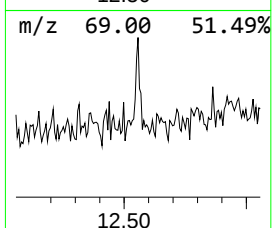
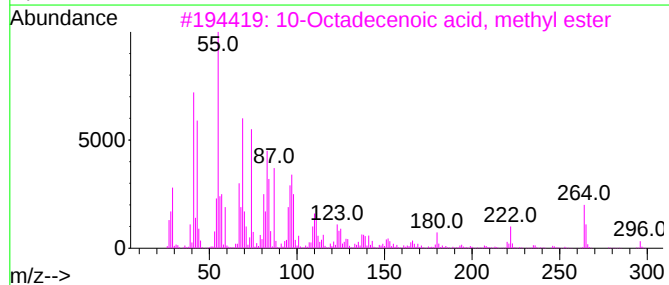
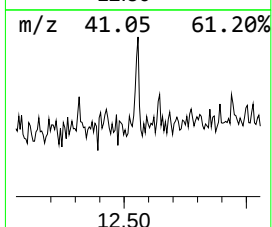
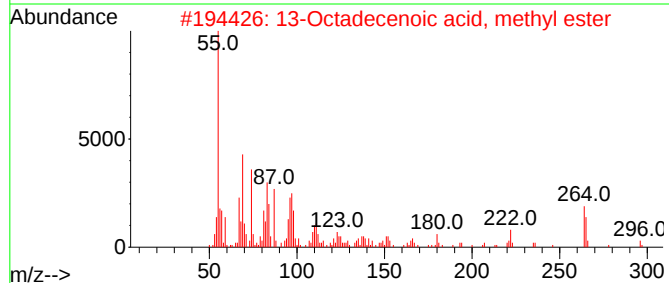
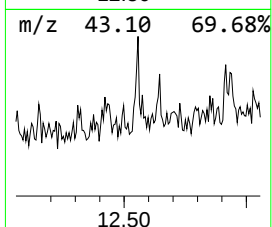
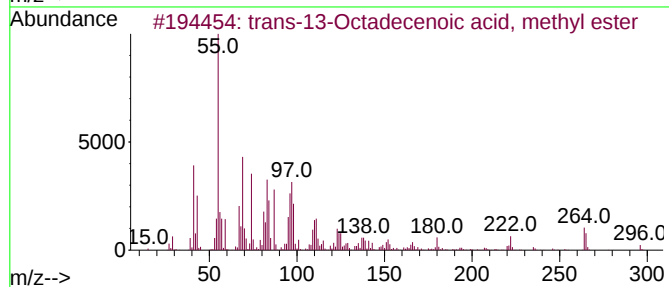
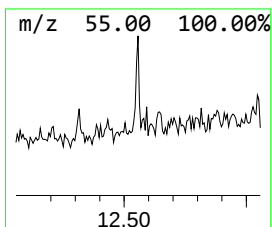
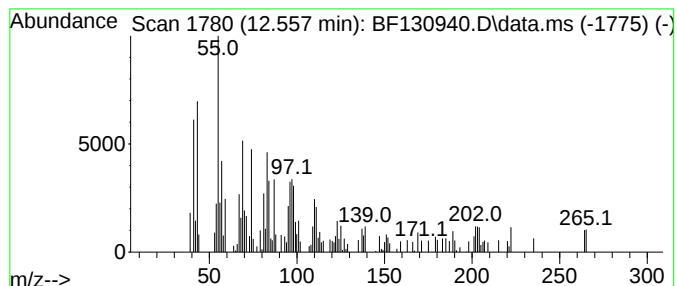
Instrument :
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ClientSampleId :
S-2-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 trans-13-Octadecenoic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.557	2.39 ng	51663	Phenanthrene-d10	11.457	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81
4	Methyl myristoleate	240	C15H28O2	056219-06-8	76
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130940.D
Acq On : 02 Nov 2022 20:35
Operator : CG\JU
Sample : N5395-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-2-103122

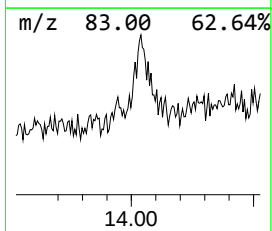
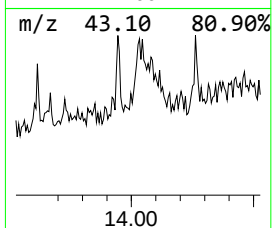
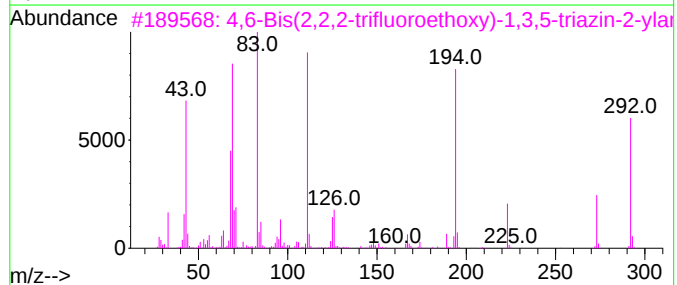
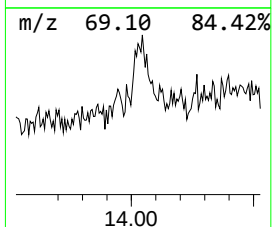
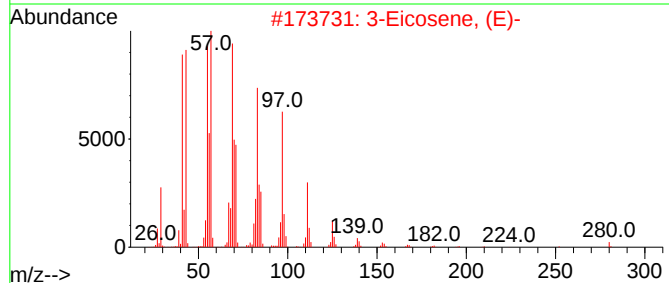
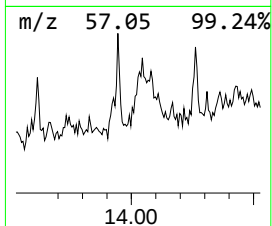
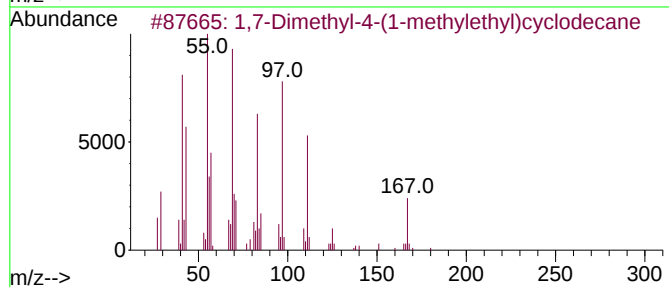
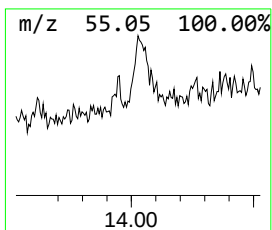
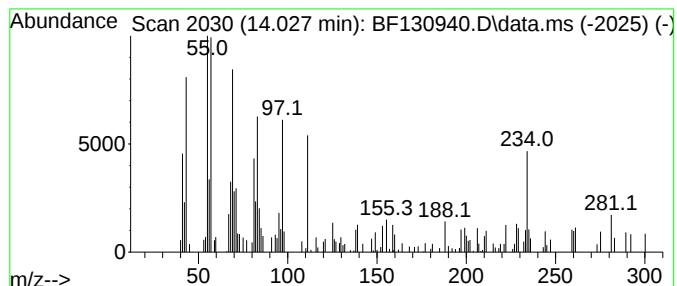
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.027 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	2.22 ng	44245	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	47
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	43
3			4,6-Bis(2,2,2-trifluoroethoxy)-1...	292	C7H6F6N4O2	301211-00-7	38
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	38
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130940.D
Acq On : 02 Nov 2022 20:35
Operator : CG\JU
Sample : N5395-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-2-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

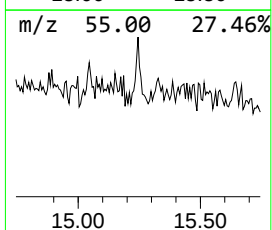
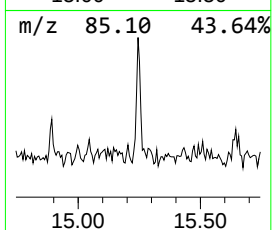
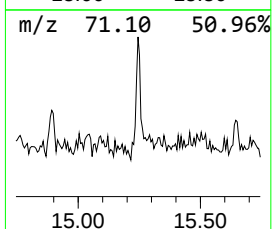
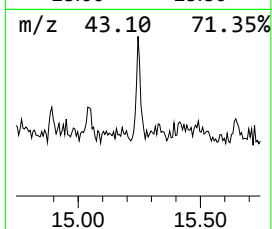
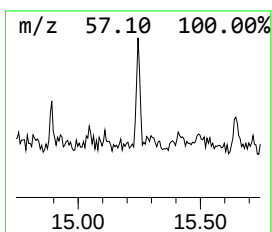
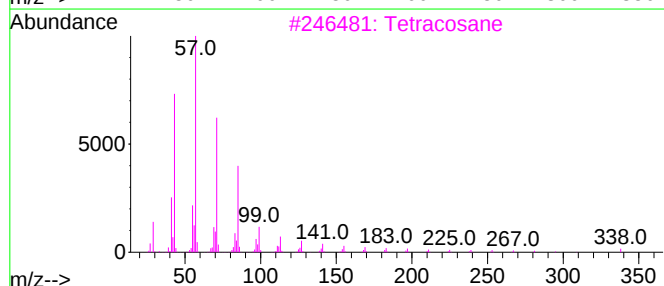
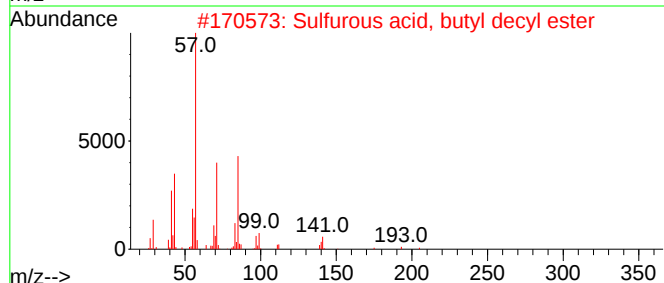
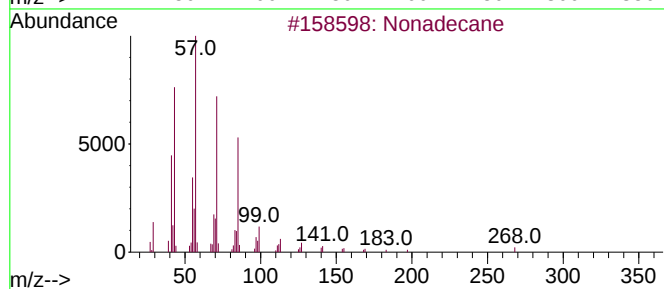
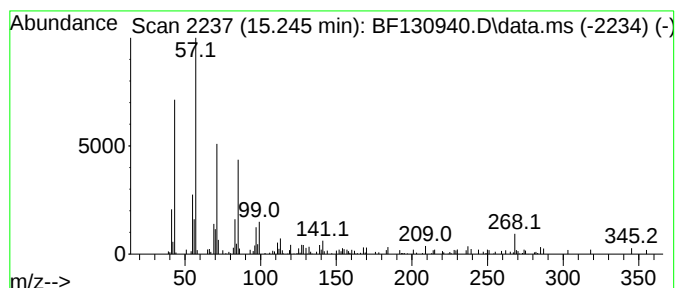
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	2.26 ng	50083	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	80
3			Tetracosane	338	C24H50	000646-31-1	72
4			Heneicosane	296	C21H44	000629-94-7	72
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130940.D
Acq On : 02 Nov 2022 20:35
Operator : CG\JU
Sample : N5395-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

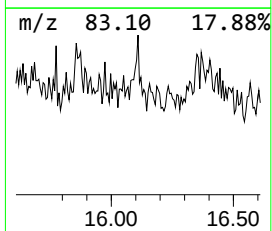
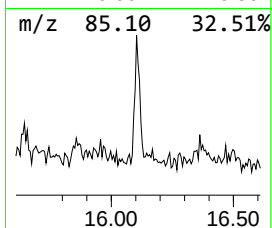
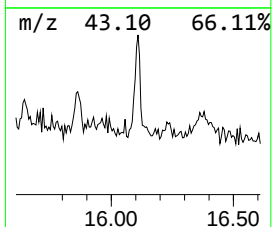
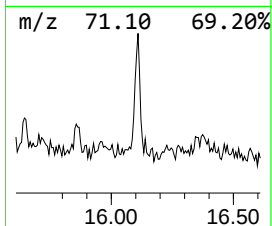
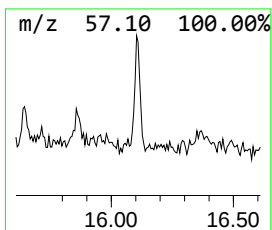
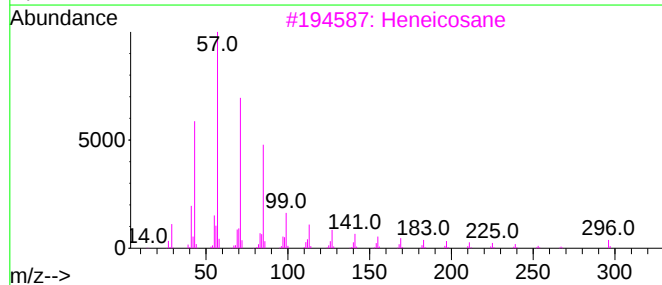
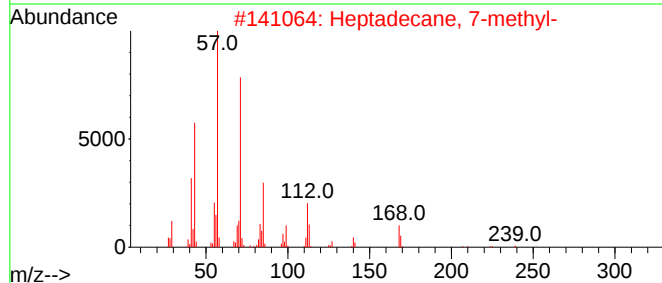
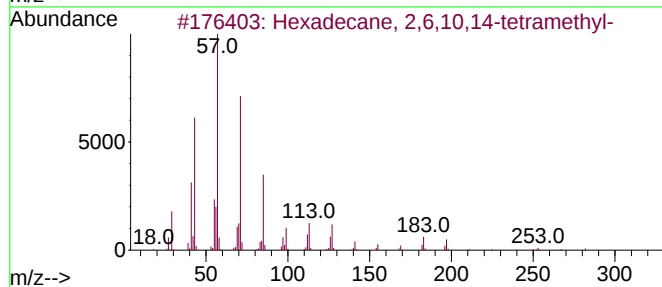
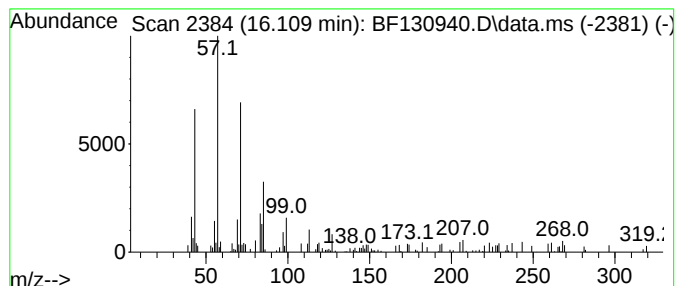
Instrument :
BNA_F
ClientSampleId :
S-2-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.110	2.54 ng	56352	Perylene-d12	15.621	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
2	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	64
3	Heneicosane	296	C21H44	000629-94-7	64
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	64
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130940.D
Acq On : 02 Nov 2022 20:35
Operator : CG\JU
Sample : N5395-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-2-103122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
Butane, 2-metho...	2.228	23.7	ng	501154	1	6.922	422688	20.0
Propane, 1,1-di...	2.340	2.0	ng	42542	1	6.922	422688	20.0
2-Pentanone, 4-...	5.151	19.9	ng	420800	1	6.922	422688	20.0
Ethanol, 1-(2-b...	8.104	9.0	ng	241683	2	8.210	538128	20.0
trans-13-Octade...	12.557	2.4	ng	51663	4	11.457	433122	20.0
unknown14.027	14.027	2.2	ng	44245	5	14.110	399316	20.0
Nonadecane	15.245	2.3	ng	50083	6	15.621	443977	20.0
Hexadecane, 2,6...	16.110	2.5	ng	56352	6	15.621	443977	20.0