

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135279.D
 Acq On : 15 Sep 2023 15:08
 Operator : CG\JU
 Sample : 04409-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1(0-2)COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs : 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	488	493	500	rVB	59507	81582	4.01%	0.473%
2	5.387	557	561	571	rBV	1867645	1928054	94.87%	11.188%
3	6.398	729	733	747	rVB	1880303	1918482	94.40%	11.133%
4	6.592	763	766	774	rBV	64997	73375	3.61%	0.426%
5	6.757	790	794	798	rBV	831277	638539	31.42%	3.705%
6	7.322	885	890	893	rBV	1263872	1179824	58.06%	6.846%
7	8.033	1007	1011	1015	rBV	1044887	884256	43.51%	5.131%
8	9.116	1190	1195	1198	rBV	2356577	2032223	100.00%	11.793%
9	9.233	1210	1215	1224	rBV	385642	347912	17.12%	2.019%
10	9.386	1236	1241	1245	rBV5	24830	25032	1.23%	0.145%
11	9.792	1306	1310	1314	rVB	1147721	929284	45.73%	5.393%
12	9.998	1341	1345	1348	rBV4	25937	30534	1.50%	0.177%
13	10.457	1414	1423	1427	rBV3	18423	43173	2.12%	0.251%
14	10.586	1441	1445	1448	rBV	1431183	1210127	59.55%	7.022%
15	10.874	1487	1494	1498	rBV4	16651	28932	1.42%	0.168%
16	11.286	1560	1564	1567	rBV	1153391	910944	44.83%	5.286%
17	11.357	1570	1576	1580	rVB6	24614	26967	1.33%	0.156%
18	11.686	1629	1632	1637	rVB	25378	23842	1.17%	0.138%
19	11.821	1650	1655	1666	rBV	377857	476757	23.46%	2.767%
20	11.969	1677	1680	1684	rBV	35412	43546	2.14%	0.253%
21	12.010	1685	1687	1698	rVB10	24719	53857	2.65%	0.313%
22	12.398	1751	1753	1756	rVB	66273	50813	2.50%	0.295%
23	12.504	1769	1771	1775	rBV	46970	48644	2.39%	0.282%
24	12.610	1784	1789	1800	rBV	172760	235705	11.60%	1.368%
25	12.733	1808	1810	1813	rVB	43758	34112	1.68%	0.198%
26	12.880	1831	1835	1839	rBV	1724172	1574038	77.45%	9.134%
27	13.368	1910	1918	1928	rBV	473568	514885	25.34%	2.988%
28	13.445	1929	1931	1937	rVB4	17273	27614	1.36%	0.160%
29	13.804	1987	1992	2002	rBV5	71820	173687	8.55%	1.008%
30	13.945	2010	2016	2019	rBV	615761	629838	30.99%	3.655%
31	14.115	2041	2045	2049	rBV	38821	43363	2.13%	0.252%
32	14.421	2093	2097	2101	rBV	70997	67806	3.34%	0.393%
33	14.727	2146	2149	2155	rVB	61572	60644	2.98%	0.352%
34	14.798	2159	2161	2165	rVB2	21287	22994	1.13%	0.133%
35	15.062	2203	2206	2210	rBV	47721	56645	2.79%	0.329%
36	15.351	2251	2255	2259	rBV	16836	29255	1.44%	0.170%

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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-BF091123.M
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37	15.409	2260	2265	2269	rVV	535691	654417	32.20%	3.797%
38	15.445	2269	2271	2278	rVB3	41196	50923	2.51%	0.295%
39	15.886	2343	2346	2352	rVB2	32654	43740	2.15%	0.254%
40	16.392	2430	2432	2437	rVB3	18985	26495	1.30%	0.154%

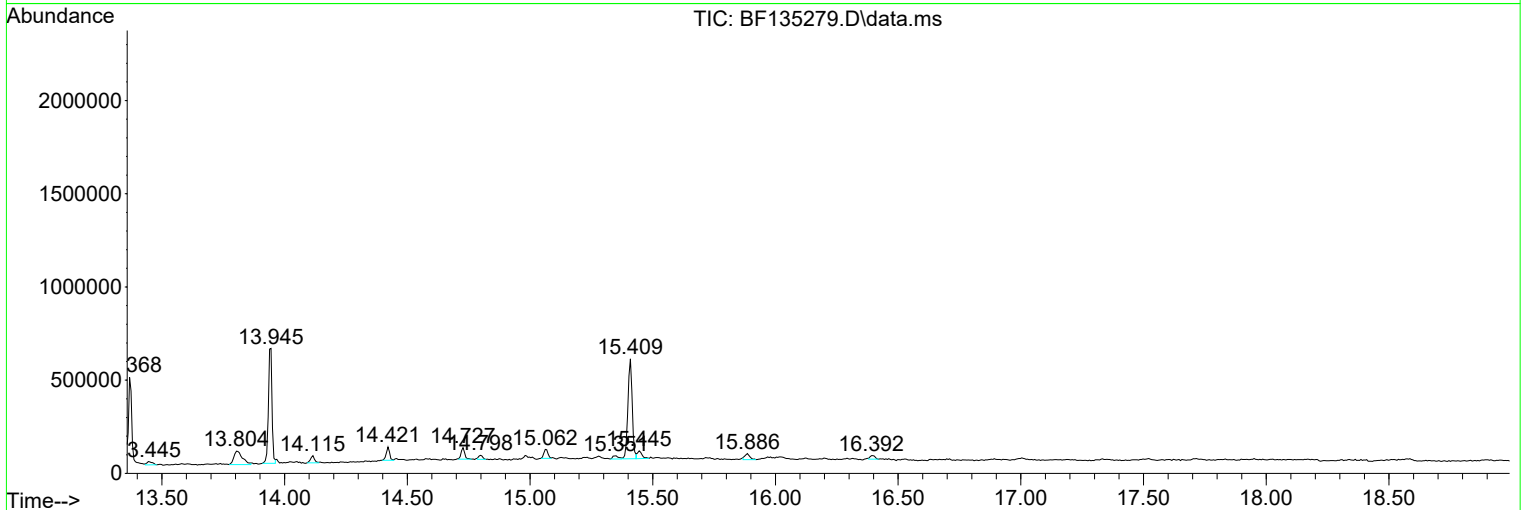
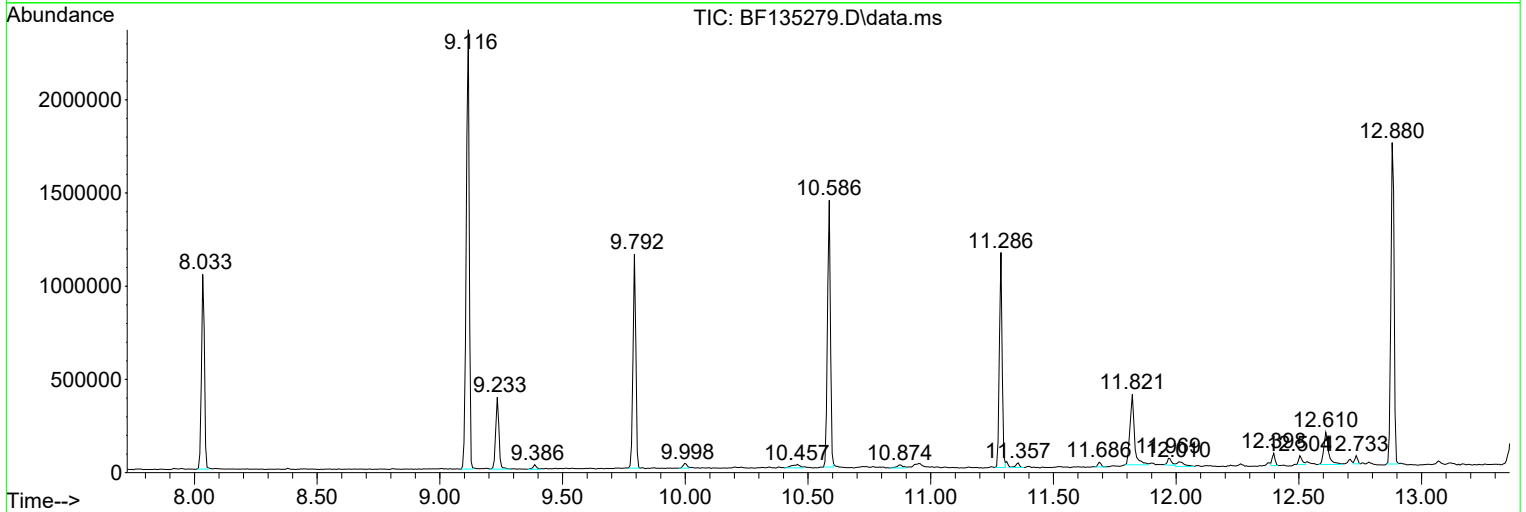
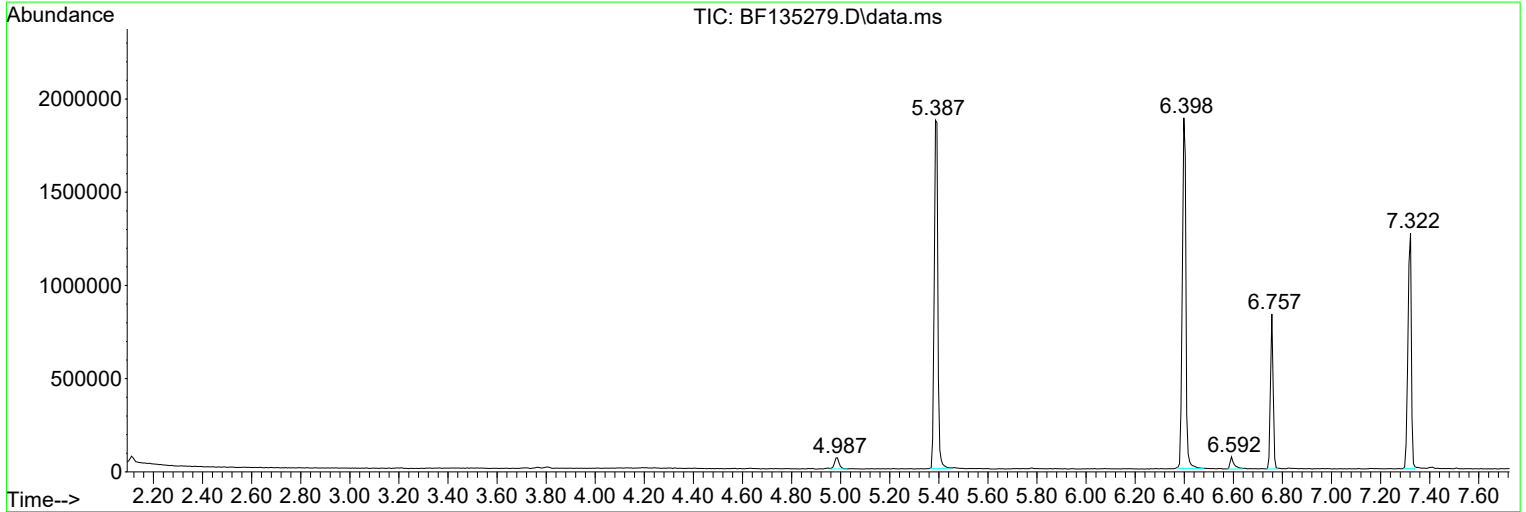
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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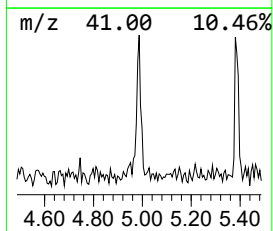
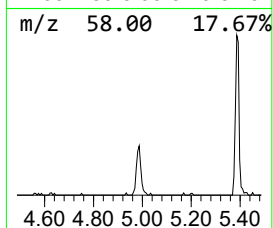
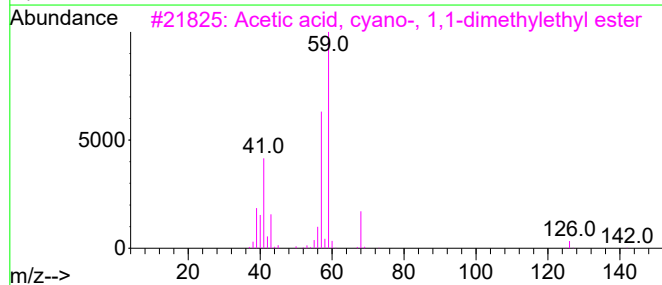
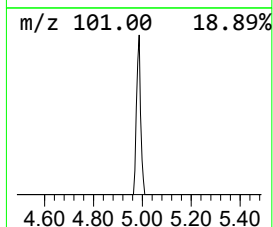
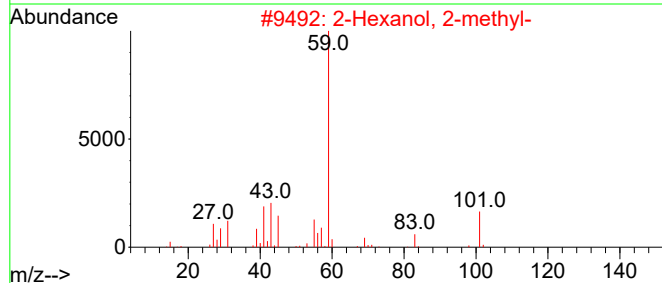
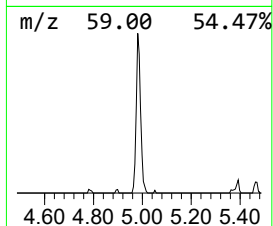
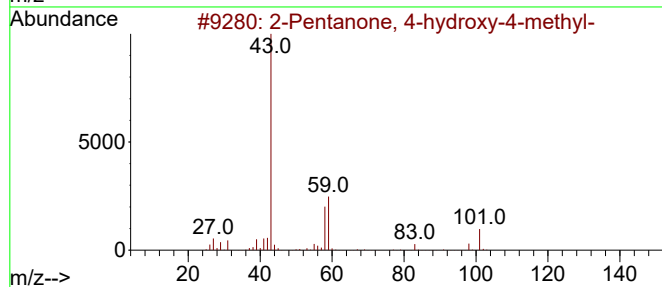
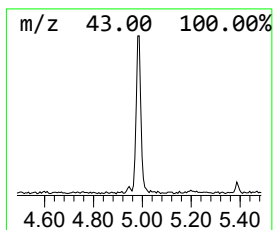
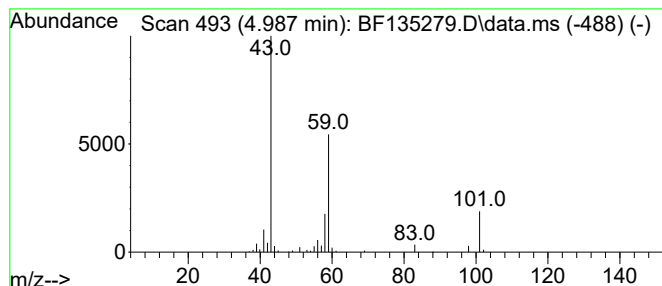
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	2.56 ng	81582	1,4-Dichlorobenzene-d4	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5		2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23



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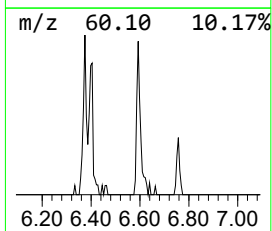
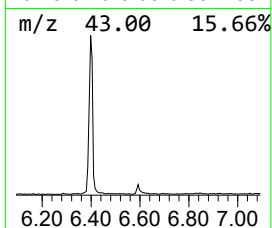
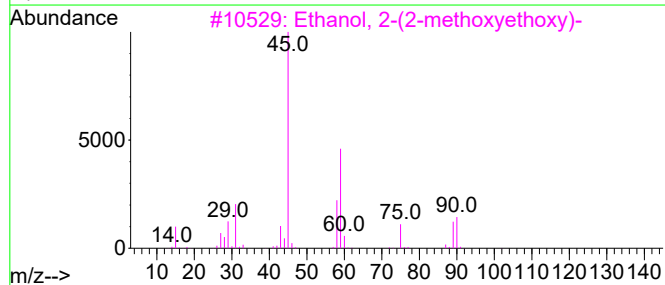
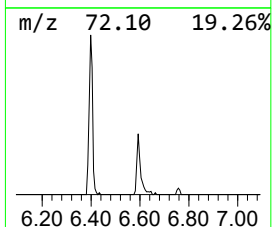
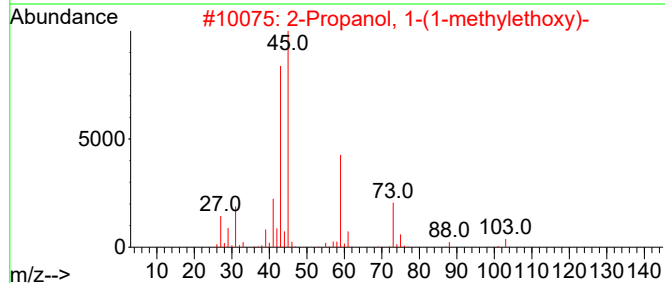
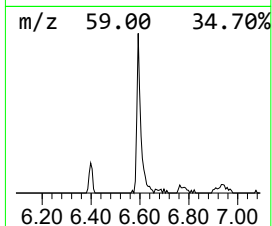
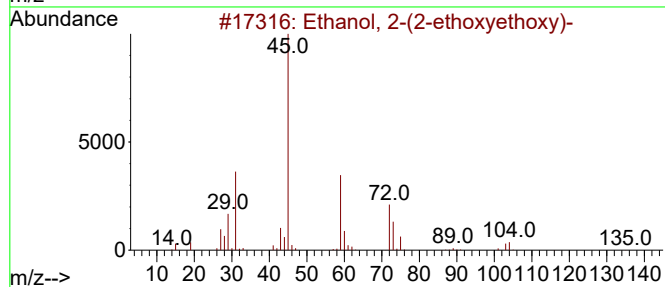
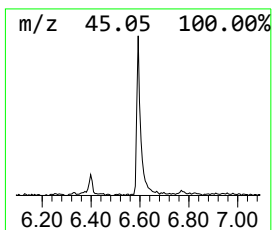
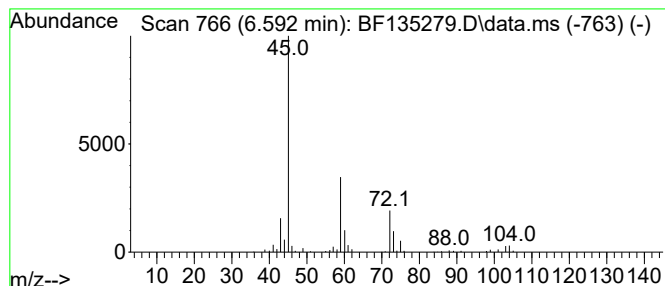
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	2.30 ng	73375	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	37
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37



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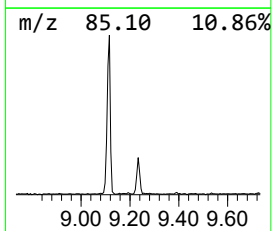
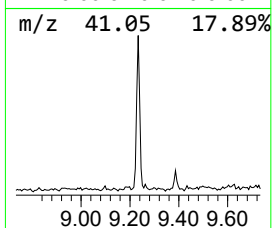
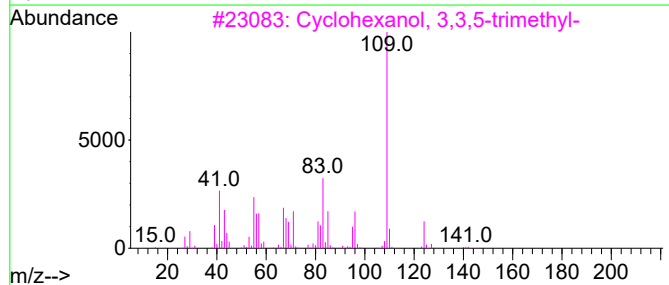
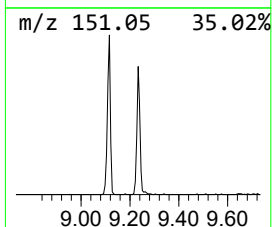
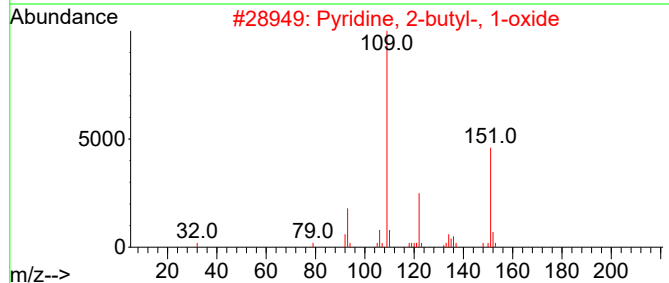
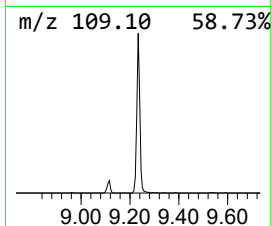
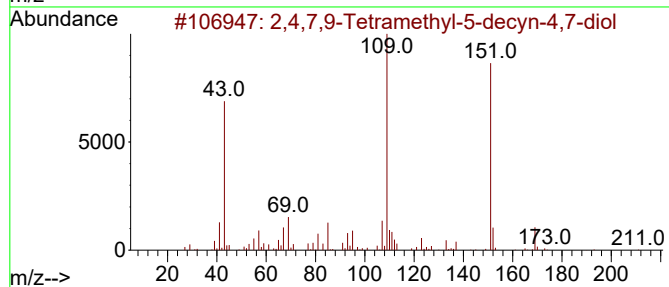
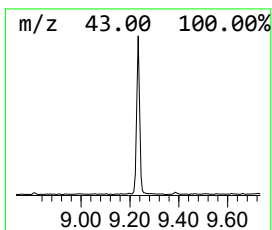
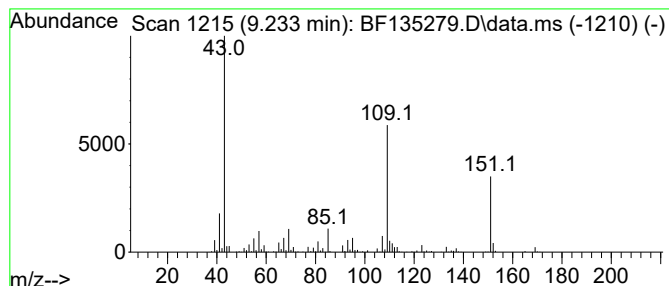
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.233	7.49 ng	347912	Acenaphthene-d10	9.792

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2		Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3		Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	50
4		Metacetamol	151	C8H9NO2	000621-42-1	49
5		Acetaminophen	151	C8H9NO2	000103-90-2	47



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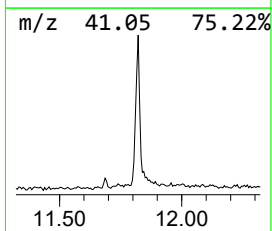
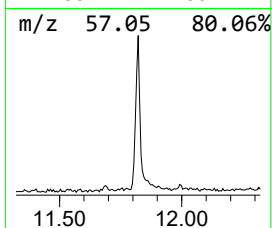
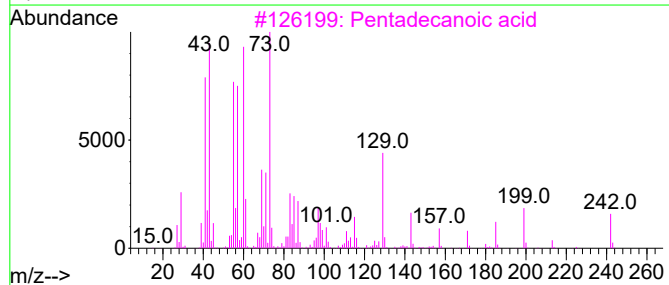
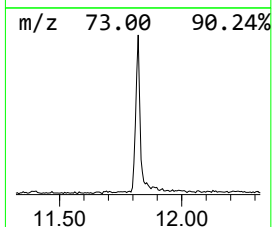
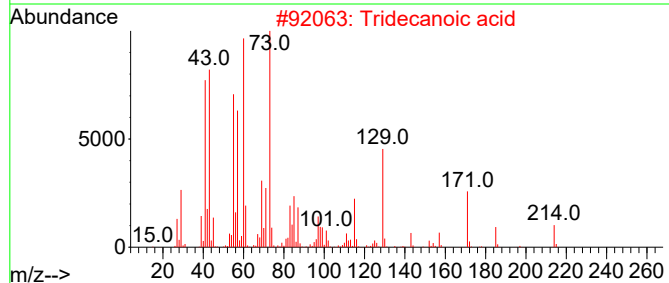
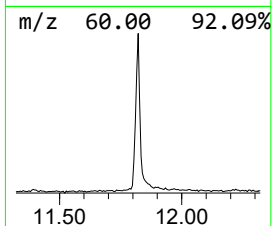
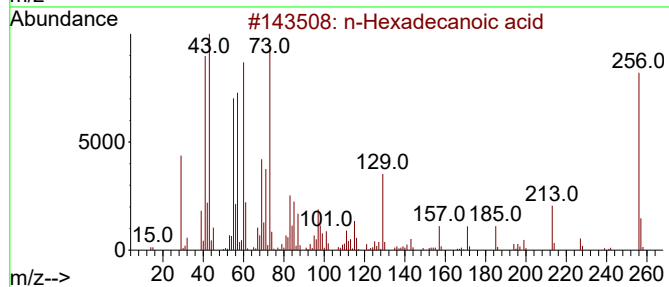
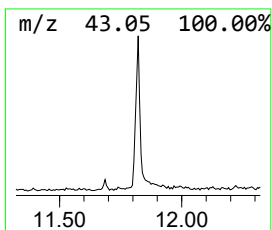
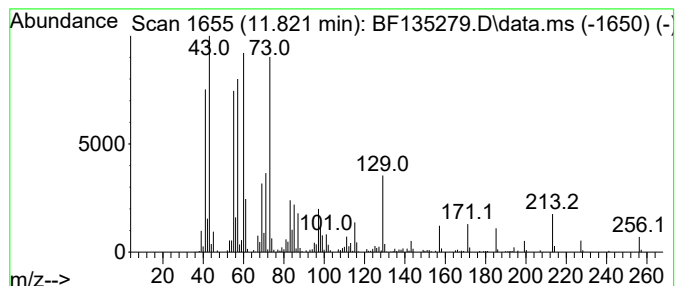
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 Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	10.47 ng	476757	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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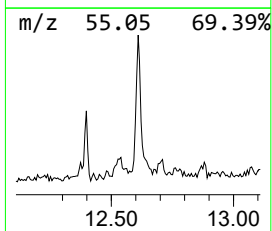
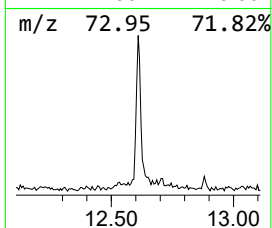
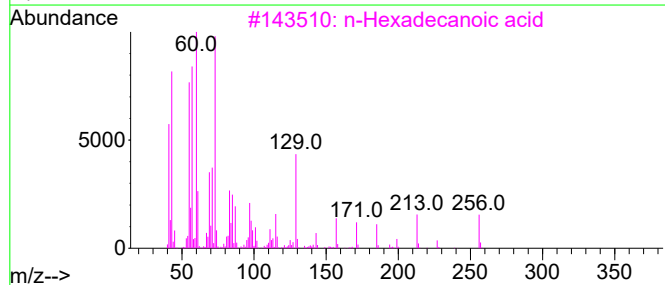
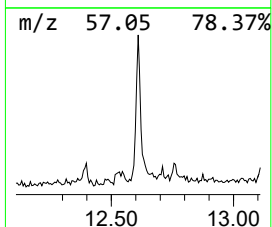
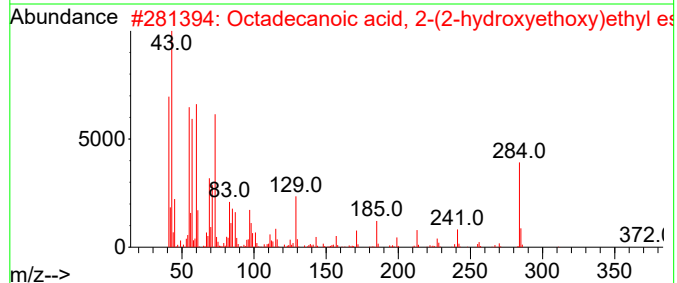
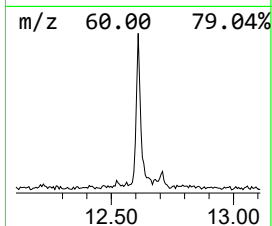
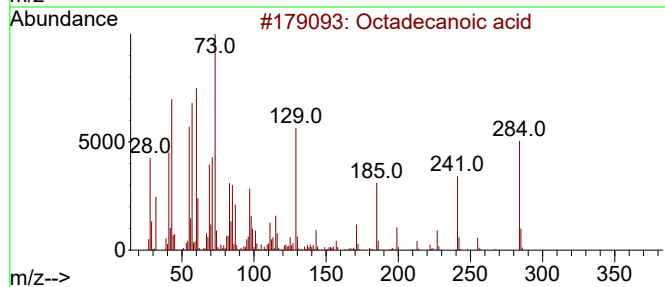
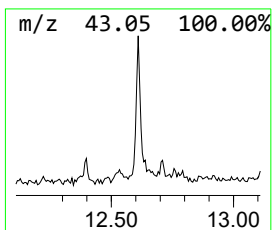
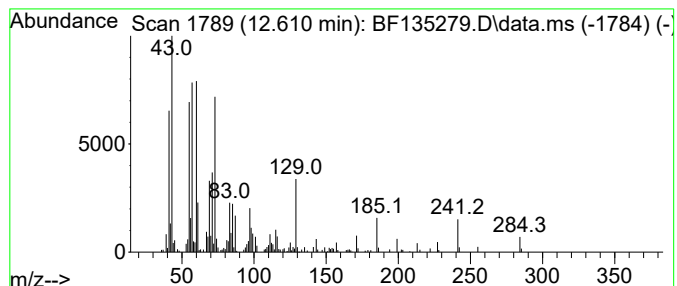
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	5.17 ng	235705	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
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 Acq On : 15 Sep 2023 15:08
 Operator : CG\JU
 Sample : 04409-01
 Misc :
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Instrument :
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 ClientSampleId :
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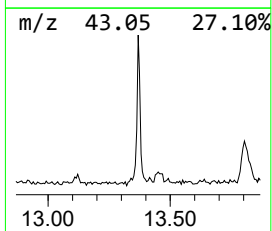
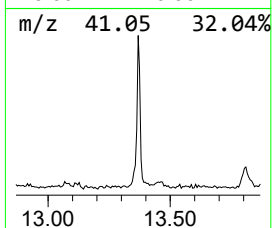
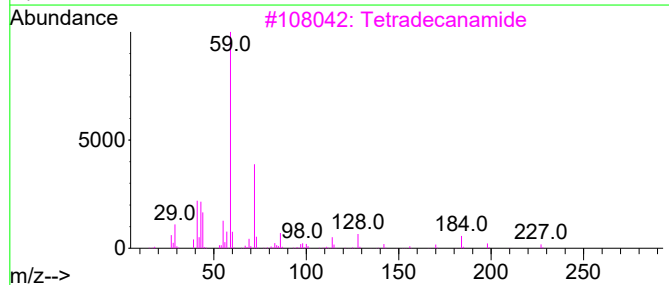
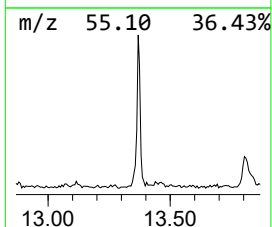
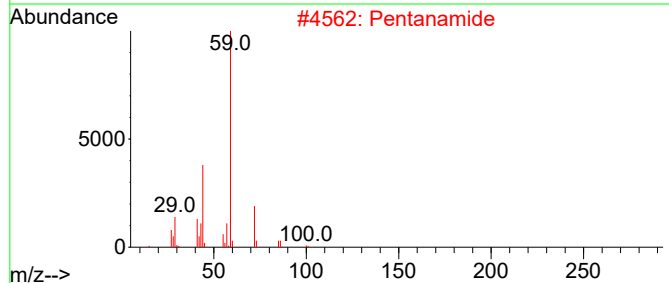
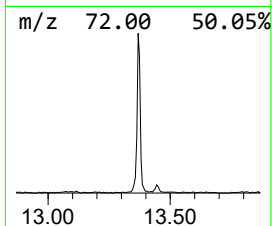
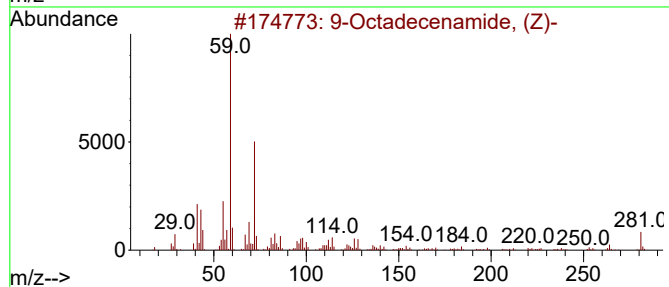
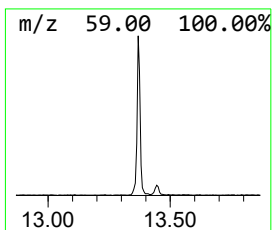
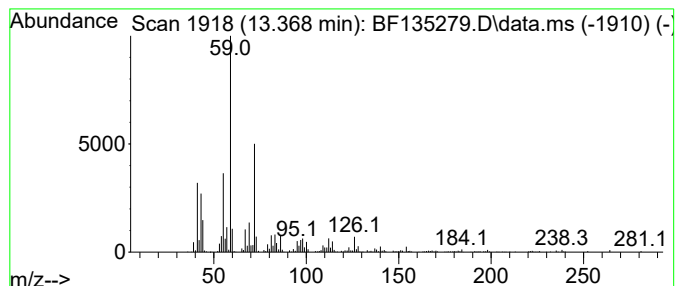
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.368	16.35 ng	514885	Chrysene-d12	13.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2		Pentanamide	101	C5H11NO	000626-97-1	64
3		Tetradecanamide	227	C14H29NO	000638-58-4	56
4		Hexadecanamide	255	C16H33NO	000629-54-9	56
5		Octadecanamide	283	C18H37NO	000124-26-5	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135279.D
 Acq On : 15 Sep 2023 15:08
 Operator : CG\JU
 Sample : 04409-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 WC-1(0-2)COMP

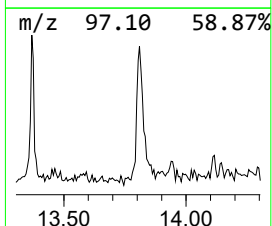
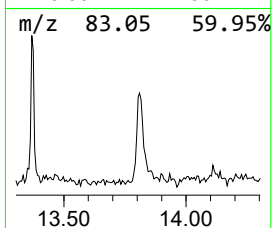
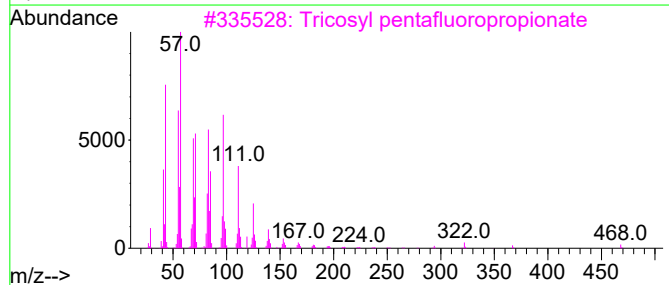
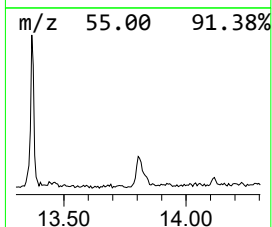
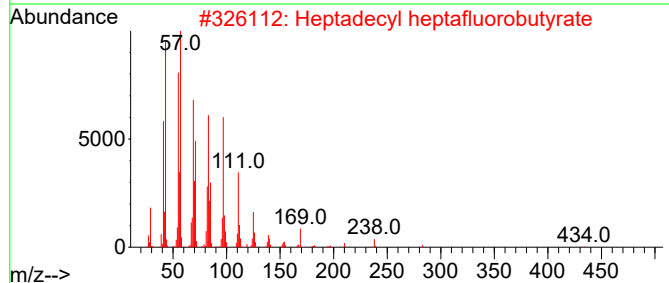
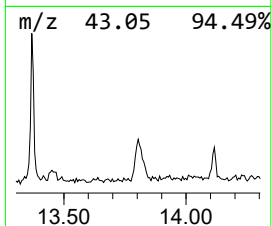
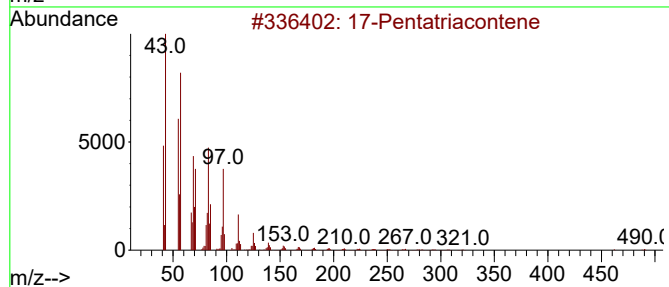
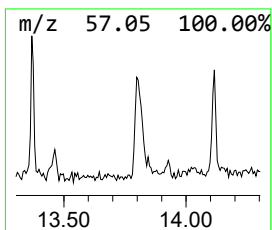
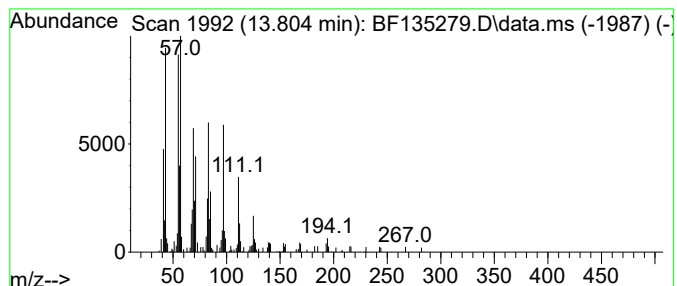
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	5.52 ng	173687	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	87
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
5			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135279.D
 Acq On : 15 Sep 2023 15:08
 Operator : CG\JU
 Sample : 04409-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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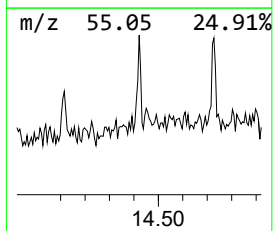
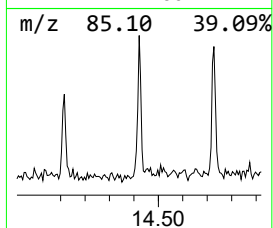
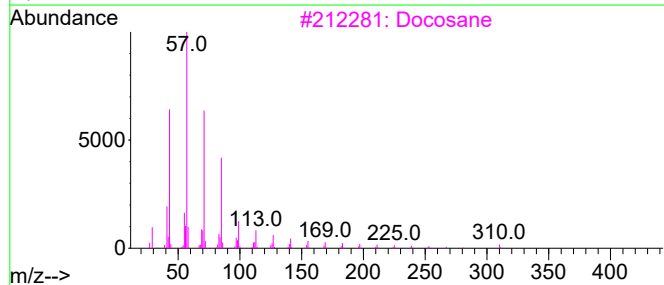
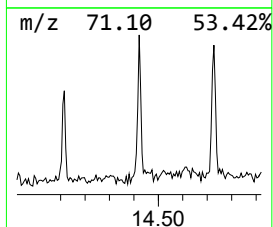
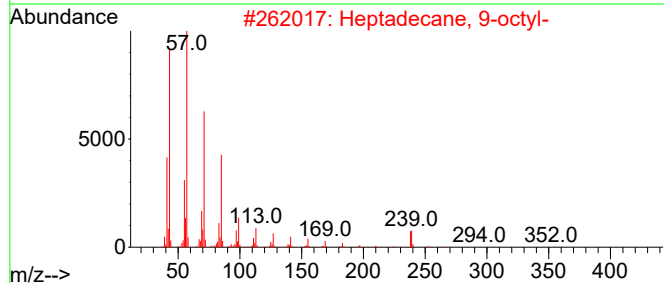
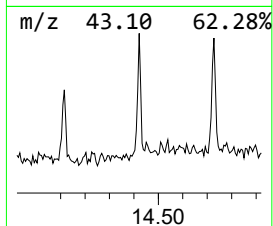
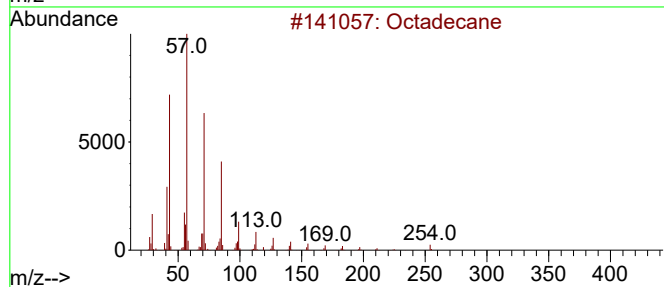
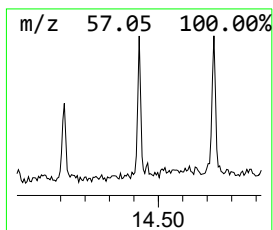
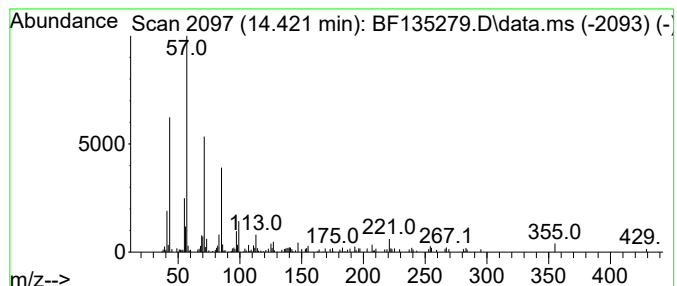
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.421	2.15 ng	67806	Chrysene-d12	13.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	93
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
3		Docosane	310	C22H46	000629-97-0	80
4		Nonadecane	268	C19H40	000629-92-5	72
5		Heneicosane	296	C21H44	000629-94-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
 Data File : BF135279.D
 Acq On : 15 Sep 2023 15:08
 Operator : CG\JU
 Sample : 04409-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
2-Pentanone, 4-...	4.987	2.6	ng	81582	1	6.757	638539	20.0
Ethanol, 2-(2-e...	6.592	2.3	ng	73375	1	6.757	638539	20.0
2,4,7,9-Tetrame...	9.233	7.5	ng	347912	3	9.792	929284	20.0
n-Hexadecanoic ...	11.822	10.5	ng	476757	4	11.286	910944	20.0
Octadecanoic acid	12.610	5.2	ng	235705	4	11.286	910944	20.0
9-Octadecenamid...	13.368	16.4	ng	514885	5	13.945	629838	20.0
17-Pentatriacon...	13.804	5.5	ng	173687	5	13.945	629838	20.0
Octadecane	14.421	2.1	ng	67806	5	13.945	629838	20.0