

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
 Data File : BF137759.D
 Acq On : 29 Apr 2024 20:32
 Operator : CG\JU
 Sample : P2294-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FOOT-PRINT-A-3

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-BF042324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.428	53	58	63	rVB	300313	378586	7.79%	1.071%
2	5.304	538	547	557	rBV	142577	149074	3.07%	0.422%
3	5.681	607	611	615	rBV	3690920	3636323	74.83%	10.292%
4	6.669	774	779	782	rBV	3907901	3731072	76.78%	10.560%
5	7.063	842	846	849	rBV	1998673	1573340	32.38%	4.453%
6	7.622	936	941	944	rBV	2928863	2441422	50.24%	6.910%
7	8.228	1041	1044	1056	rBV	482972	453166	9.33%	1.283%
8	8.345	1060	1064	1067	rBV	2632385	2080125	42.80%	5.887%
9	8.645	1111	1115	1124	rVB	113204	105656	2.17%	0.299%
10	9.422	1242	1247	1250	rBV	5292985	4859600	100.00%	13.754%
11	9.739	1297	1301	1304	rBV	213048	171613	3.53%	0.486%
12	10.104	1360	1363	1367	rBV	2572293	2214168	45.56%	6.267%
13	10.186	1373	1377	1383	rBV2	111839	157384	3.24%	0.445%
14	10.892	1493	1497	1501	rBV	2741320	2449558	50.41%	6.933%
15	11.598	1613	1617	1620	rBV	2230798	1840061	37.86%	5.208%
16	11.622	1620	1621	1625	rVB	152497	98239	2.02%	0.278%
17	12.104	1699	1703	1706	rBV	493707	414932	8.54%	1.174%
18	12.816	1821	1824	1828	rBV	303142	275670	5.67%	0.780%
19	12.892	1833	1837	1842	rBV2	95246	112914	2.32%	0.320%
20	13.051	1857	1864	1870	rBV	220825	266852	5.49%	0.755%
21	13.186	1883	1887	1890	rBV	4248528	3476121	71.53%	9.838%
22	13.616	1957	1960	1963	rBV2	161243	153252	3.15%	0.434%
23	13.645	1963	1965	1970	rVB3	54622	61379	1.26%	0.174%
24	13.745	1979	1982	1985	rBV	60776	51481	1.06%	0.146%
25	14.074	2035	2038	2050	rBV2	246358	421907	8.68%	1.194%
26	14.251	2063	2068	2071	rBV	1604996	1502406	30.92%	4.252%
27	14.274	2071	2072	2079	rVB	125942	93691	1.93%	0.265%
28	14.392	2089	2092	2094	rBV2	88930	85949	1.77%	0.243%
29	14.704	2142	2145	2147	rBV	95679	104227	2.14%	0.295%
30	15.033	2199	2201	2205	rVB	57007	55384	1.14%	0.157%
31	15.198	2226	2229	2234	rVB	148690	158474	3.26%	0.449%
32	15.345	2251	2254	2258	rBV	89960	144481	2.97%	0.409%
33	15.410	2262	2265	2270	rVB	145351	164436	3.38%	0.465%
34	15.821	2331	2335	2346	rVB	889019	1263100	25.99%	3.575%
35	16.327	2417	2421	2429	rVB	118087	186454	3.84%	0.528%

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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-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

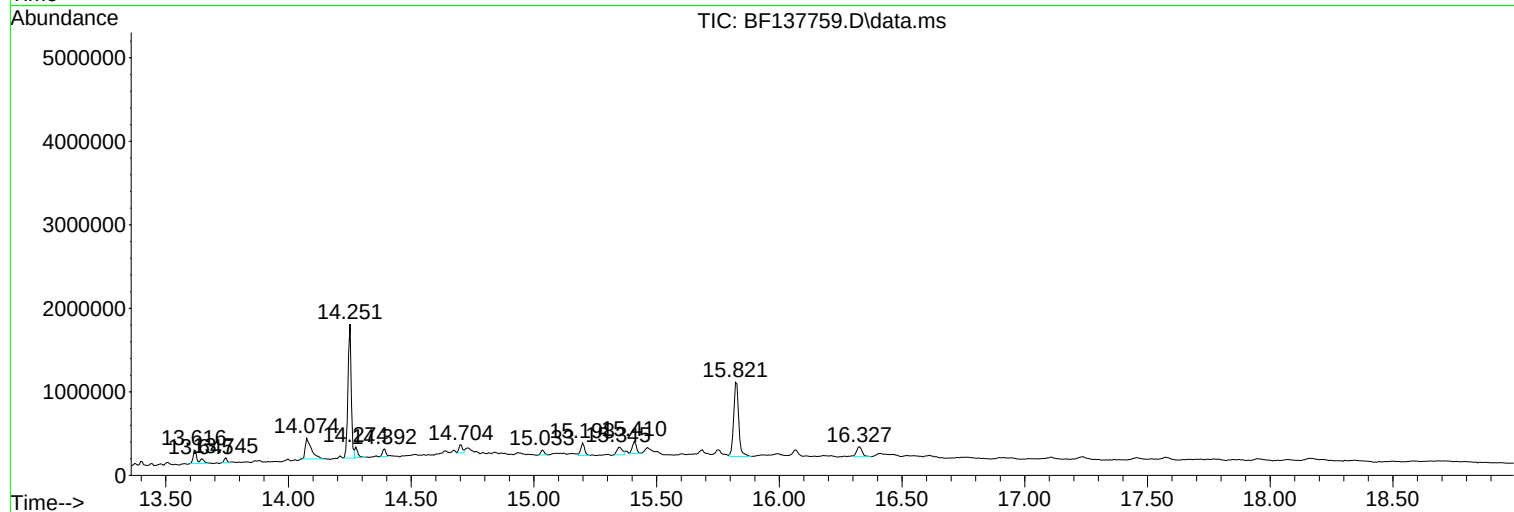
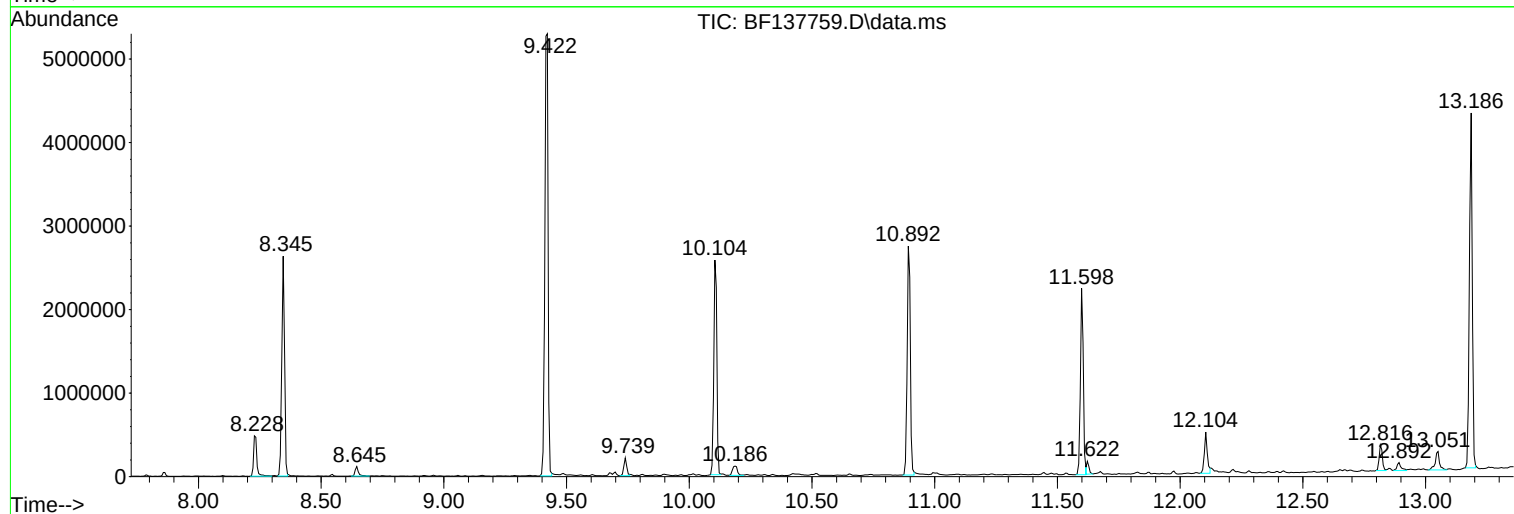
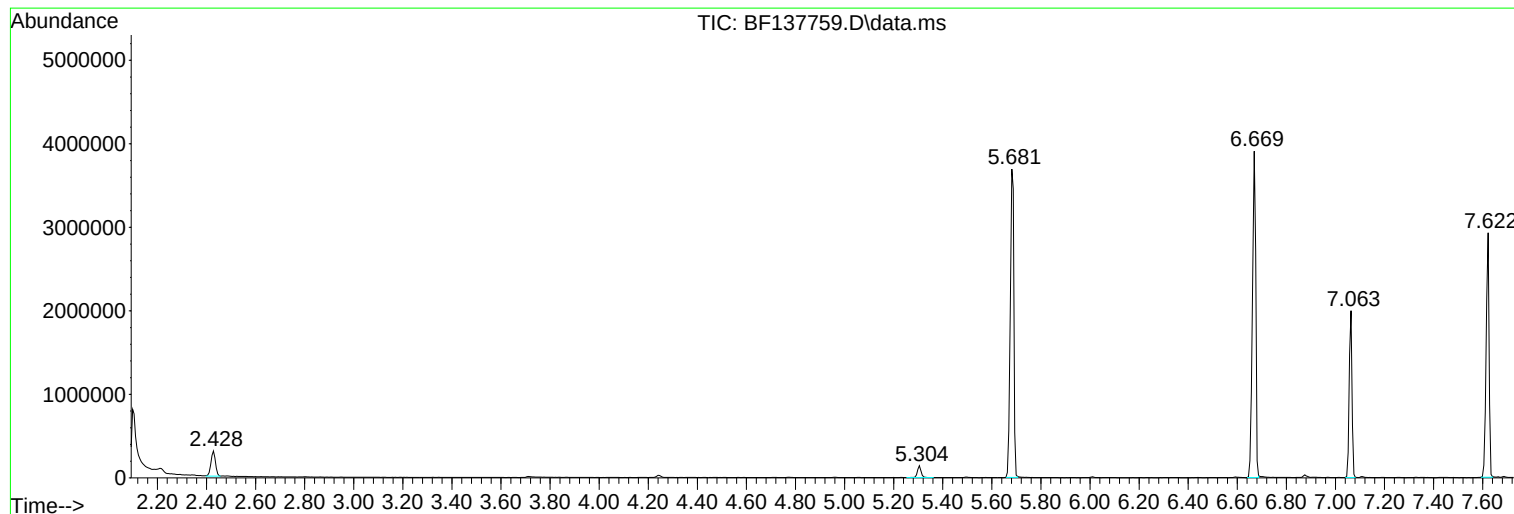
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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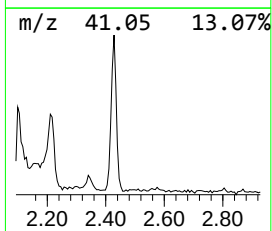
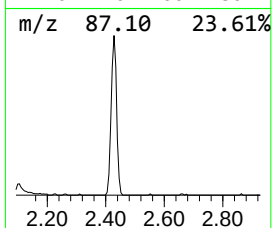
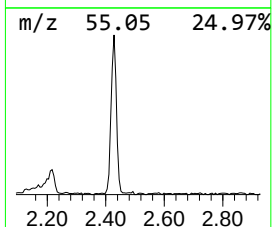
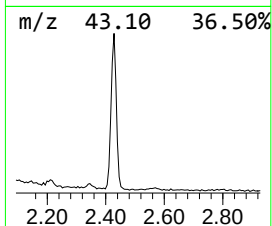
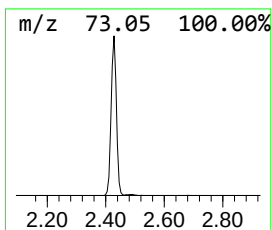
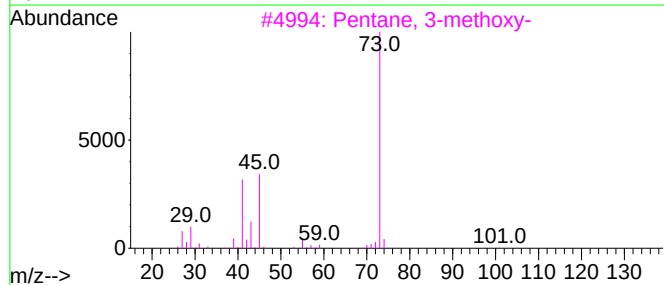
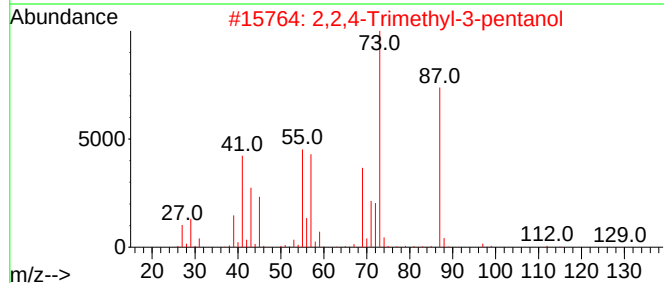
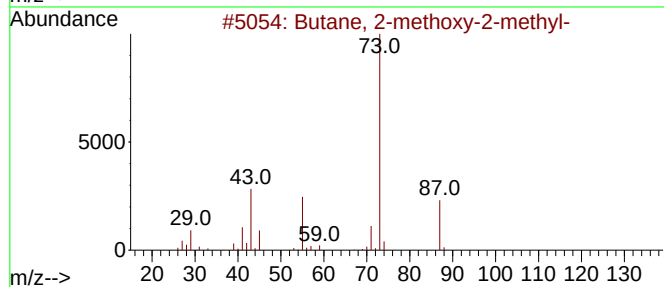
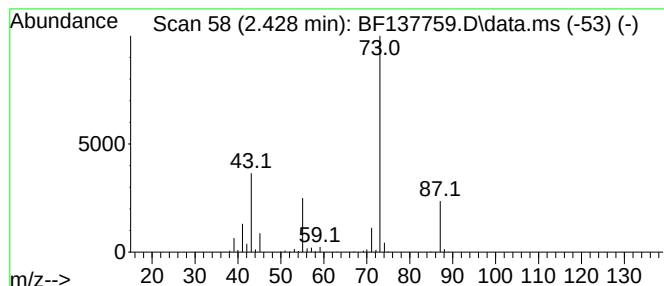
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.428	4.81 ng	378586	1,4-Dichlorobenzene-d4	7.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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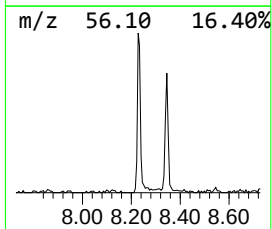
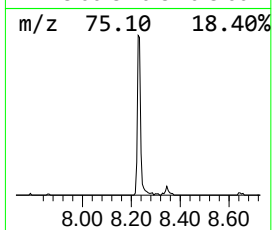
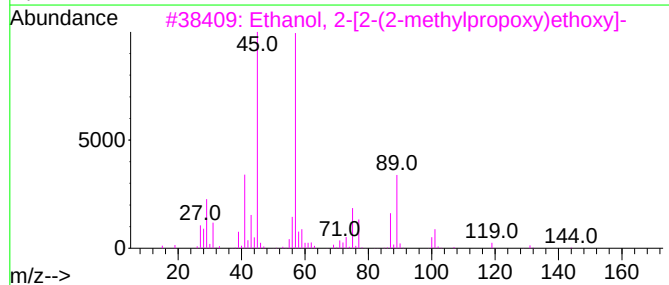
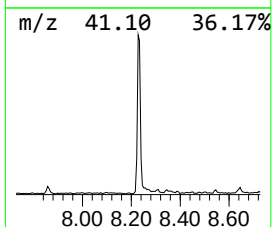
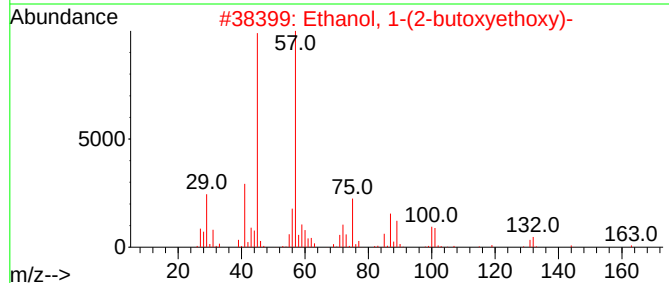
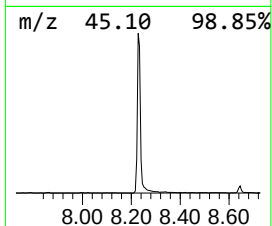
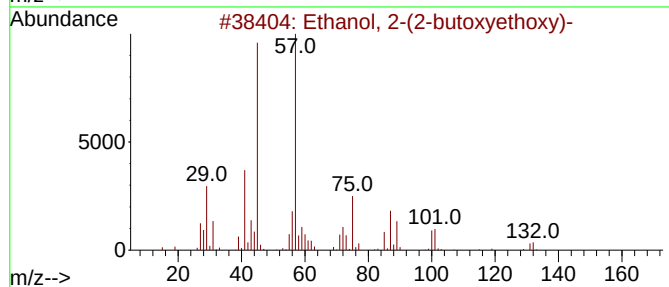
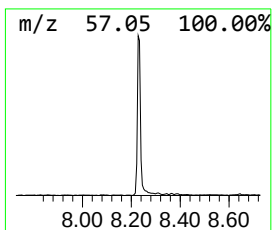
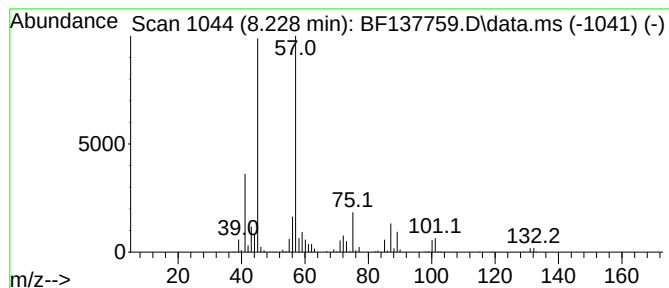
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.228	4.36 ng	453166	Naphthalene-d8	8.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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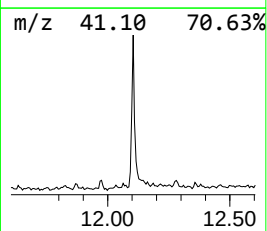
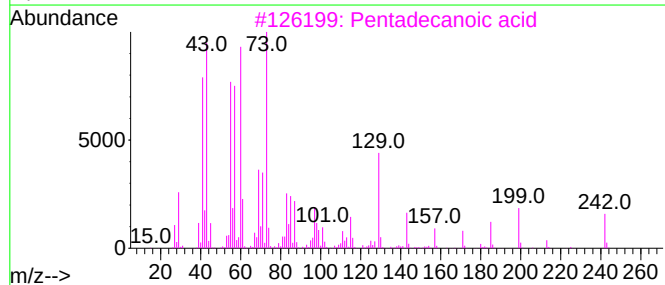
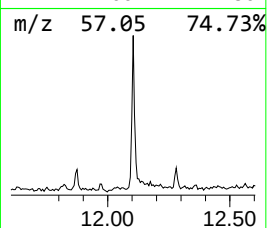
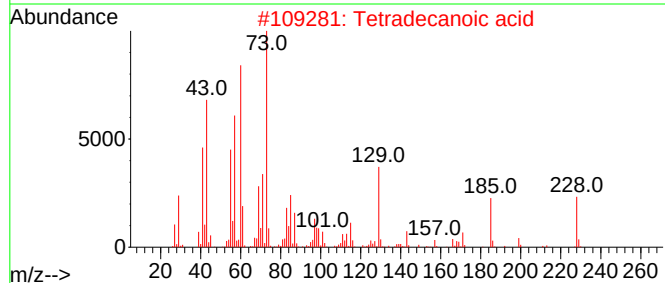
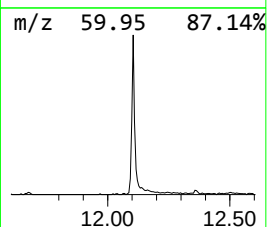
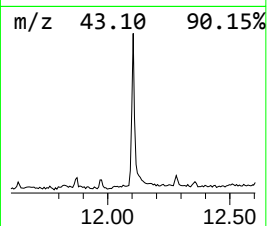
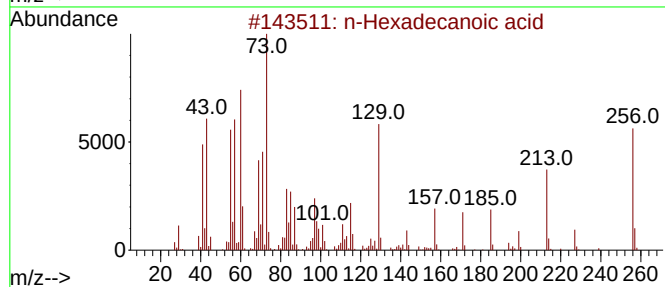
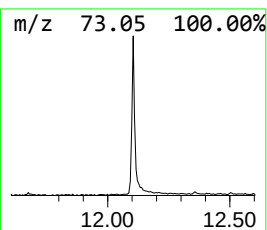
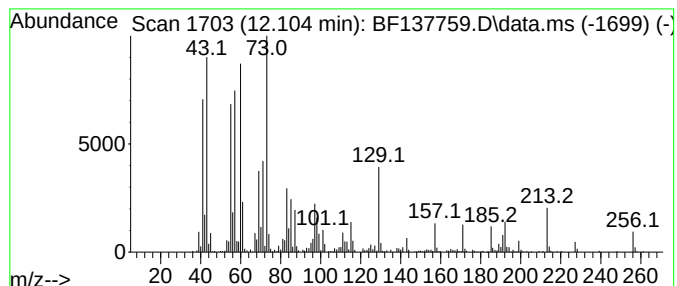
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	4.51 ng	414932	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



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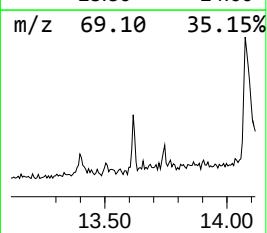
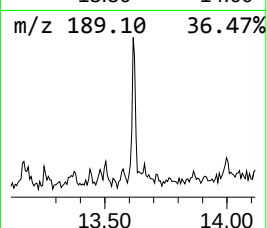
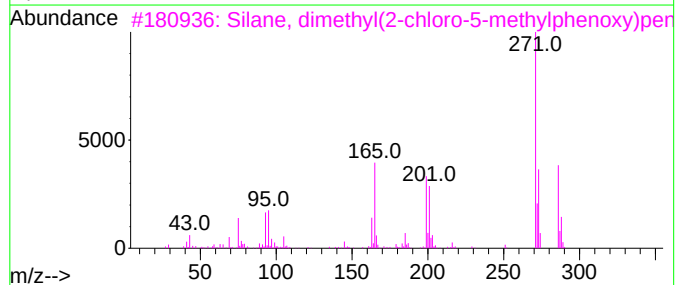
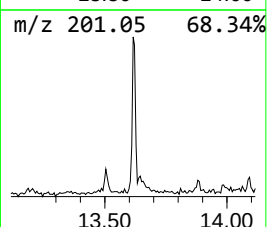
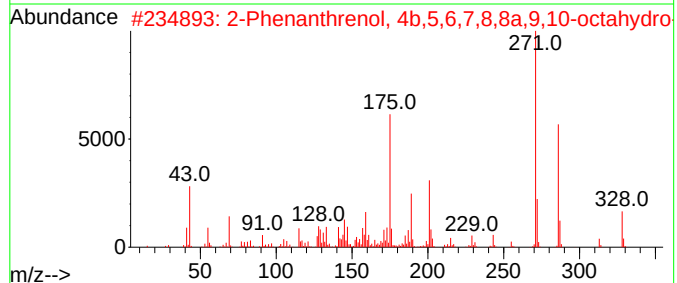
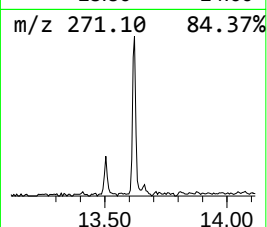
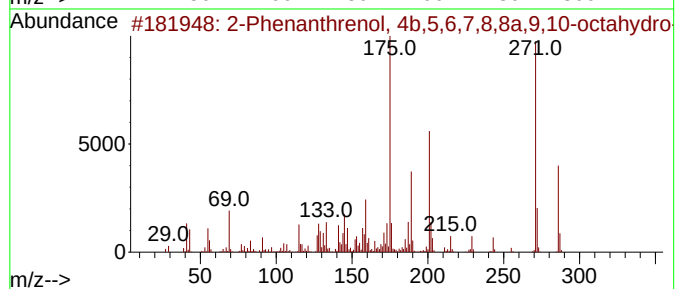
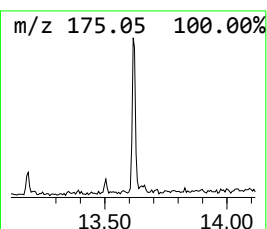
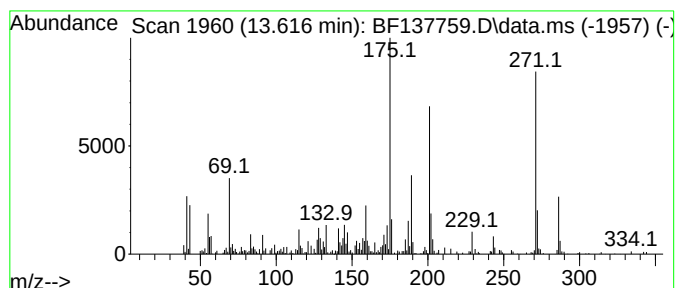
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.616	2.04 ng	153252	Chrysene-d12	14.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99		
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	87		
3	Silane, dimethyl(2-chloro-5-meth...	286	C14H23ClO2Si	1000347-54-6	35		
4	1,2-Naphthalenedione, 6-hydroxy-...	244	C15H16O3	007715-96-0	25		
5	Naphthalene, 1,2,3,4-tetrahydro-...	244	C18H28	029577-17-1	25		



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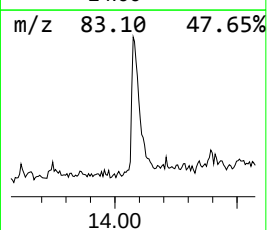
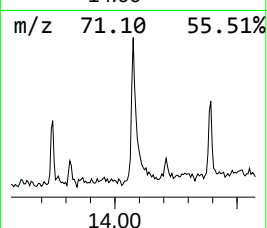
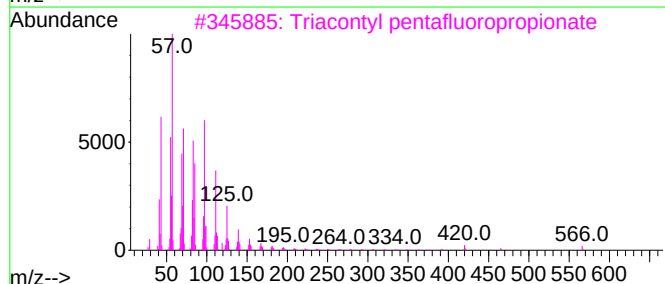
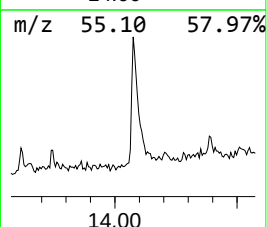
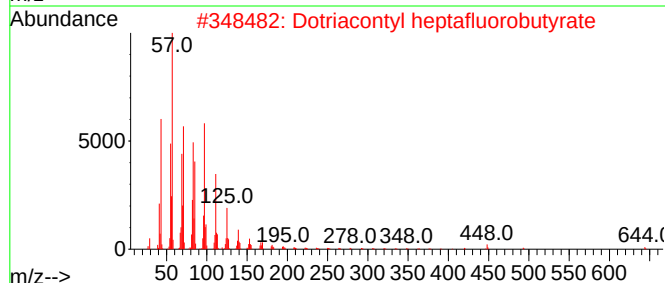
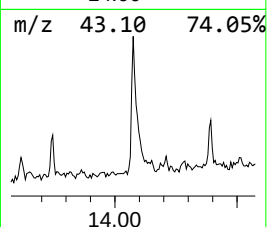
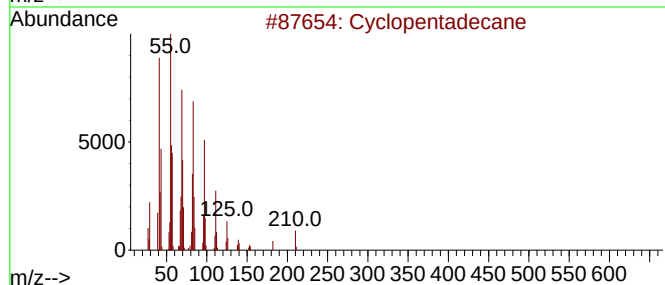
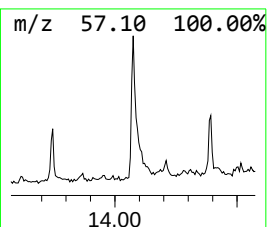
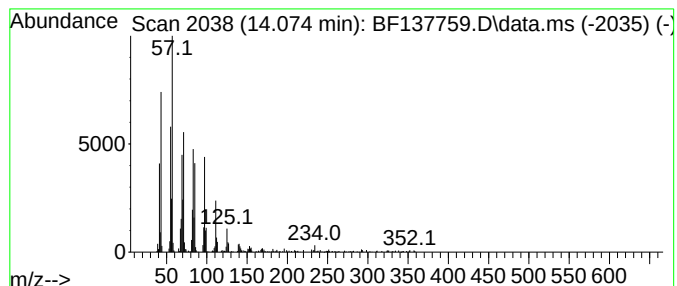
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.075	5.62 ng	421907	Chrysene-d12	14.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
3			Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
4			Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	91
5			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
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Acq On : 29 Apr 2024 20:32
Operator : CG\JU
Sample : P2294-03
Misc :
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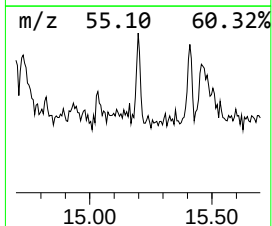
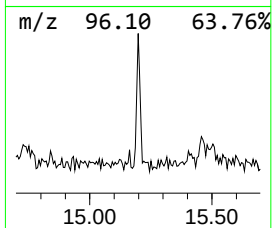
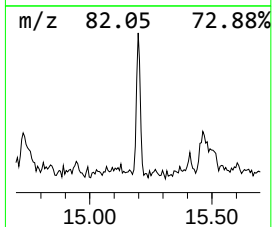
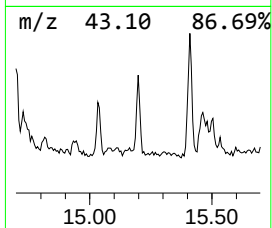
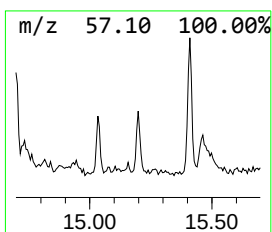
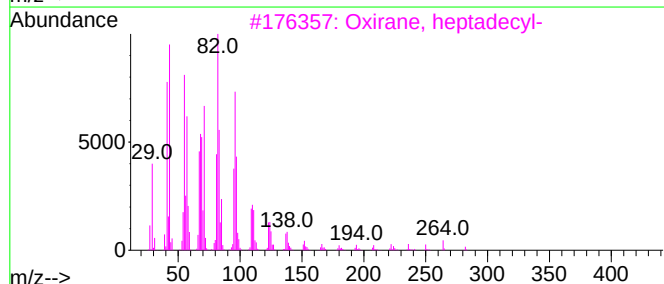
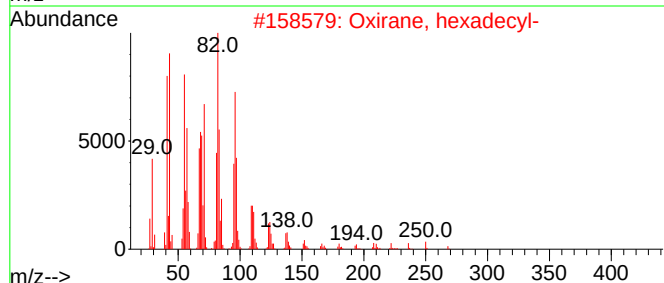
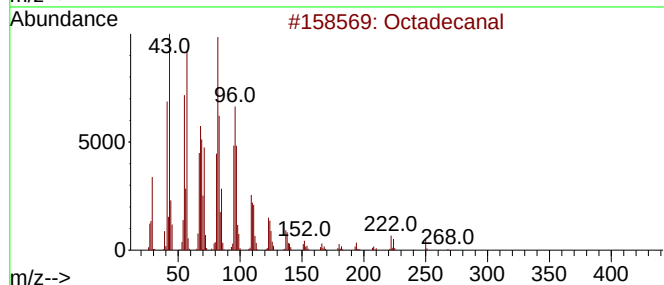
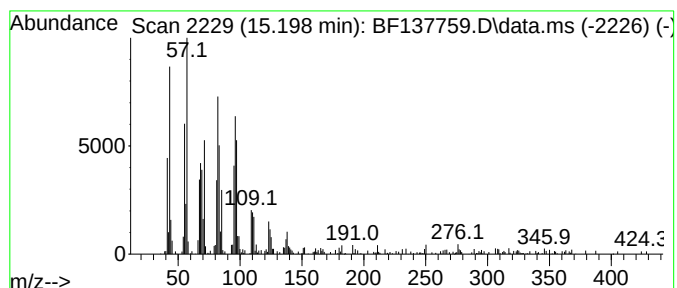
Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-A-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.198	2.51 ng	158474	Perylene-d12	15.821	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
4	Hexacosanal	380	C26H52O	026627-85-0	87
5	Ethanol, 2-(9-octadecenyl)-, ...	312	C20H40O2	005353-25-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137759.D
Acq On : 29 Apr 2024 20:32
Operator : CG\JU
Sample : P2294-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-A-3

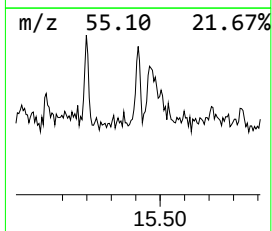
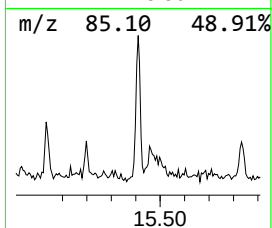
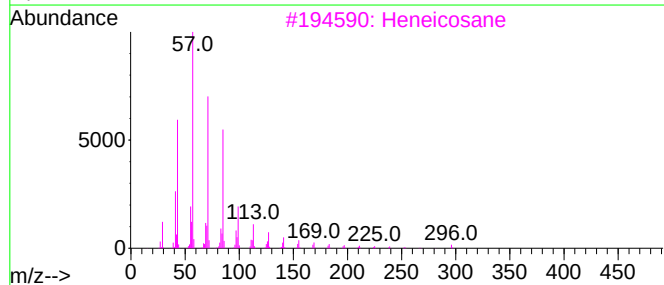
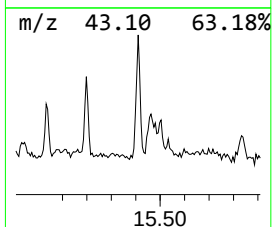
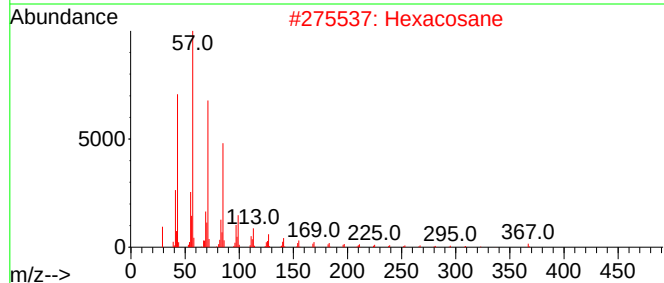
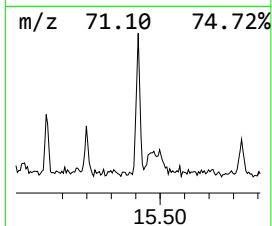
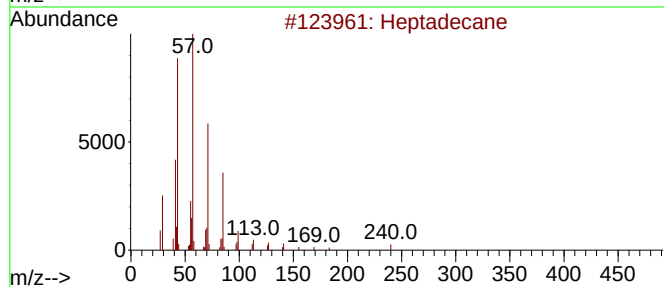
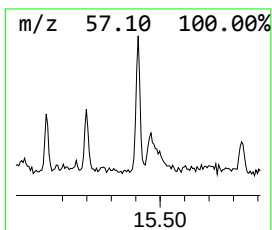
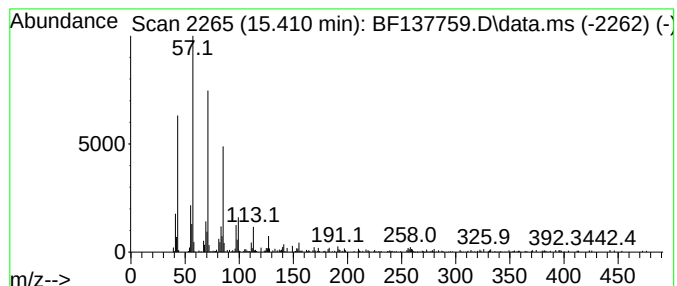
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	2.60 ng	164436	Perylene-d12	15.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137759.D
Acq On : 29 Apr 2024 20:32
Operator : CG\JU
Sample : P2294-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-A-3

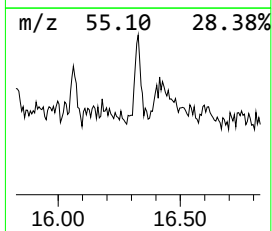
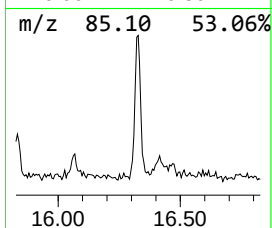
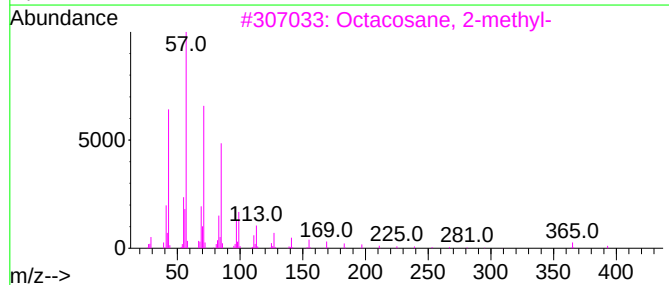
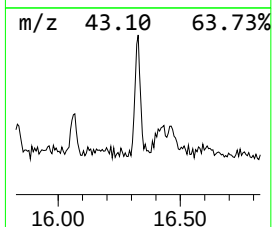
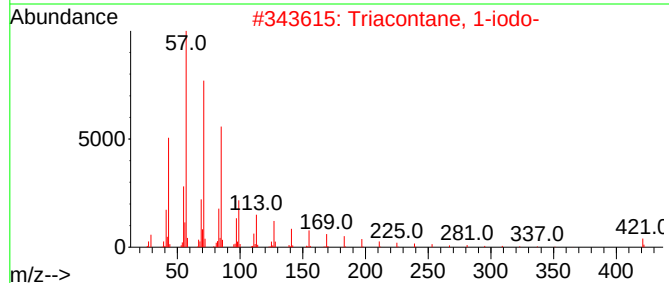
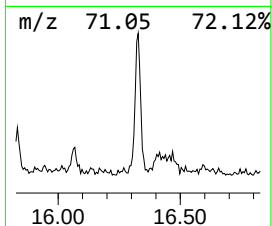
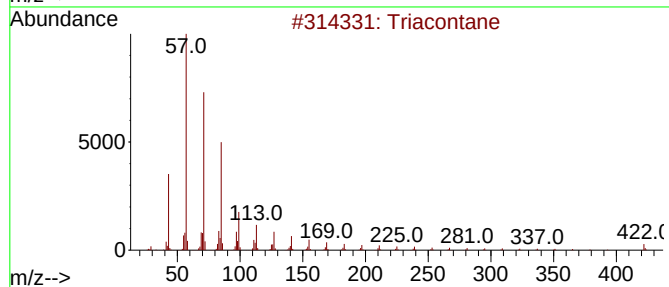
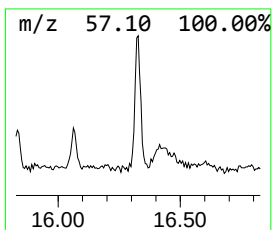
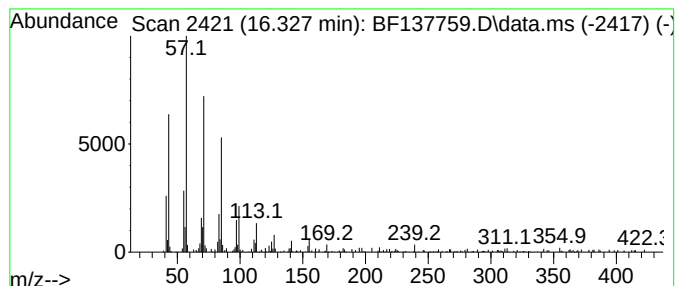
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	2.95 ng	186454	Perylene-d12	15.821

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	94
2		Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4		Octadecane	254	C18H38	000593-45-3	90
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137759.D
Acq On : 29 Apr 2024 20:32
Operator : CG\JU
Sample : P2294-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-A-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.428	4.8	ng	378586	1	7.063	1573340	20.0
Ethanol, 2-(2-b...	8.228	4.4	ng	453166	2	8.345	2080130	20.0
n-Hexadecanoic ...	12.104	4.5	ng	414932	4	11.598	1840060	20.0
2-Phenanthrenol...	13.616	2.0	ng	153252	5	14.251	1502410	20.0
Cyclopentadecane	14.075	5.6	ng	421907	5	14.251	1502410	20.0
Octadecanal	15.198	2.5	ng	158474	6	15.821	1263100	20.0
Heptadecane	15.410	2.6	ng	164436	6	15.821	1263100	20.0
Triacontane	16.327	3.0	ng	186454	6	15.821	1263100	20.0