

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136824.D
 Acq On : 29 Dec 2023 12:36
 Operator : CG\JU
 Sample : 06017-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB32-1-20231222-10.0-11.0

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	12	17	20	rBV2	12401	21077	1.25%	0.160%
2	2.216	20	22	28	rVB2	15405	21465	1.27%	0.163%
3	3.516	228	243	248	rBV2	18311	42869	2.54%	0.326%
4	3.652	255	266	274	rBV	16008	30180	1.79%	0.229%
5	3.846	291	299	301	rBV2	19301	28353	1.68%	0.215%
6	3.875	301	304	308	rVB3	18904	25110	1.49%	0.191%
7	3.987	318	323	329	rVB	25980	40774	2.42%	0.310%
8	4.128	337	347	352	rBV2	20839	32391	1.92%	0.246%
9	4.557	413	420	425	rBV5	12222	20367	1.21%	0.155%
10	4.940	482	485	491	rVB2	29060	36032	2.14%	0.274%
11	5.028	495	500	506	rBV	24377	34390	2.04%	0.261%
12	5.210	527	531	533	rBV2	16330	18347	1.09%	0.139%
13	5.240	533	536	540	rVB3	10995	17301	1.03%	0.131%
14	5.293	540	545	547	rBV2	37173	37742	2.24%	0.287%
15	5.316	547	549	552	rVB	48899	38850	2.30%	0.295%
16	5.387	559	561	564	rBV	41722	40035	2.37%	0.304%
17	5.428	564	568	571	rBV	1614766	1433075	84.92%	10.882%
18	5.569	587	592	597	rBV4	13983	25099	1.49%	0.191%
19	5.851	637	640	644	rBV2	13873	20170	1.20%	0.153%
20	5.934	648	654	656	rBV	18679	23326	1.38%	0.177%
21	6.034	668	671	674	rBV2	27070	26321	1.56%	0.200%
22	6.222	698	703	705	rBV3	22895	29227	1.73%	0.222%
23	6.246	705	707	709	rVV	49449	40955	2.43%	0.311%
24	6.281	709	713	716	rVB2	45206	56991	3.38%	0.433%
25	6.316	716	719	721	rBV	39657	35332	2.09%	0.268%
26	6.369	726	728	731	rBV	39637	35553	2.11%	0.270%
27	6.428	734	738	741	rBV	1579159	1466085	86.88%	11.132%
28	6.781	795	798	803	rVB	513205	404733	23.98%	3.073%
29	6.857	809	811	814	rVB2	21615	19252	1.14%	0.146%
30	6.898	814	818	820	rBV2	19019	20994	1.24%	0.159%
31	6.957	826	828	831	rVB	37914	27935	1.66%	0.212%
32	7.028	837	840	842	rBV	40676	30813	1.83%	0.234%
33	7.051	842	844	847	rVB	27956	21939	1.30%	0.167%
34	7.116	853	855	859	rVB	40049	33136	1.96%	0.252%
35	7.163	859	863	867	rBV2	25221	23769	1.41%	0.180%
36	7.198	867	869	875	rVV2	26428	34253	2.03%	0.260%

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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-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	7.310	881	888	890	rBV	103354	103008	6.10%	0.782%
38	7.345	890	894	897	rVB	1044416	948679	56.22%	7.204%
39	7.545	926	928	931	rVB	57131	41708	2.47%	0.317%
40	7.598	935	937	944	rVB3	15549	22494	1.33%	0.171%
41	7.663	944	948	950	rBV2	20322	22407	1.33%	0.170%
42	7.734	957	960	964	rVB4	41961	54262	3.22%	0.412%
43	7.793	968	970	975	rVV3	58706	63423	3.76%	0.482%
44	7.928	987	993	996	rVB2	23693	23427	1.39%	0.178%
45	8.057	1010	1015	1021	rVV	619857	567956	33.66%	4.313%
46	8.104	1021	1023	1027	rVB2	23363	25326	1.50%	0.192%
47	8.440	1077	1080	1083	rVB2	22582	22627	1.34%	0.172%
48	9.134	1194	1198	1202	rBV	1761911	1687536	100.00%	12.814%
49	9.816	1310	1314	1323	rBV	718276	581351	34.45%	4.414%
50	9.916	1326	1331	1338	rVB5	11356	17048	1.01%	0.129%
51	10.610	1445	1449	1452	rBV	1198980	1050523	62.25%	7.977%
52	11.310	1564	1568	1571	rBV	710487	608154	36.04%	4.618%
53	11.375	1575	1579	1584	rVB3	25775	23125	1.37%	0.176%
54	11.845	1655	1659	1669	rBV	172454	197653	11.71%	1.501%
55	11.951	1673	1677	1680	rVB	48318	43664	2.59%	0.332%
56	12.051	1691	1694	1698	rVB	50133	39285	2.33%	0.298%
57	12.163	1707	1713	1716	rBV2	61142	53369	3.16%	0.405%
58	12.569	1775	1782	1786	rBV3	15890	17353	1.03%	0.132%
59	12.633	1789	1793	1798	rBV4	19052	27878	1.65%	0.212%
60	12.904	1835	1839	1842	rBV	1780751	1534776	90.95%	11.654%
61	13.039	1857	1862	1866	rVB	40881	37484	2.22%	0.285%
62	13.810	1989	1993	1997	rBV	21142	20832	1.23%	0.158%
63	13.869	1997	2003	2015	rBV7	34383	135587	8.03%	1.030%
64	13.963	2015	2019	2028	rVB	504325	454202	26.92%	3.449%
65	14.439	2097	2100	2103	rVB	18860	17664	1.05%	0.134%
66	14.821	2161	2165	2168	rBV	28680	31612	1.87%	0.240%
67	15.086	2207	2210	2216	rVB3	13539	18042	1.07%	0.137%
68	15.445	2266	2271	2280	rBV	294992	382866	22.69%	2.907%

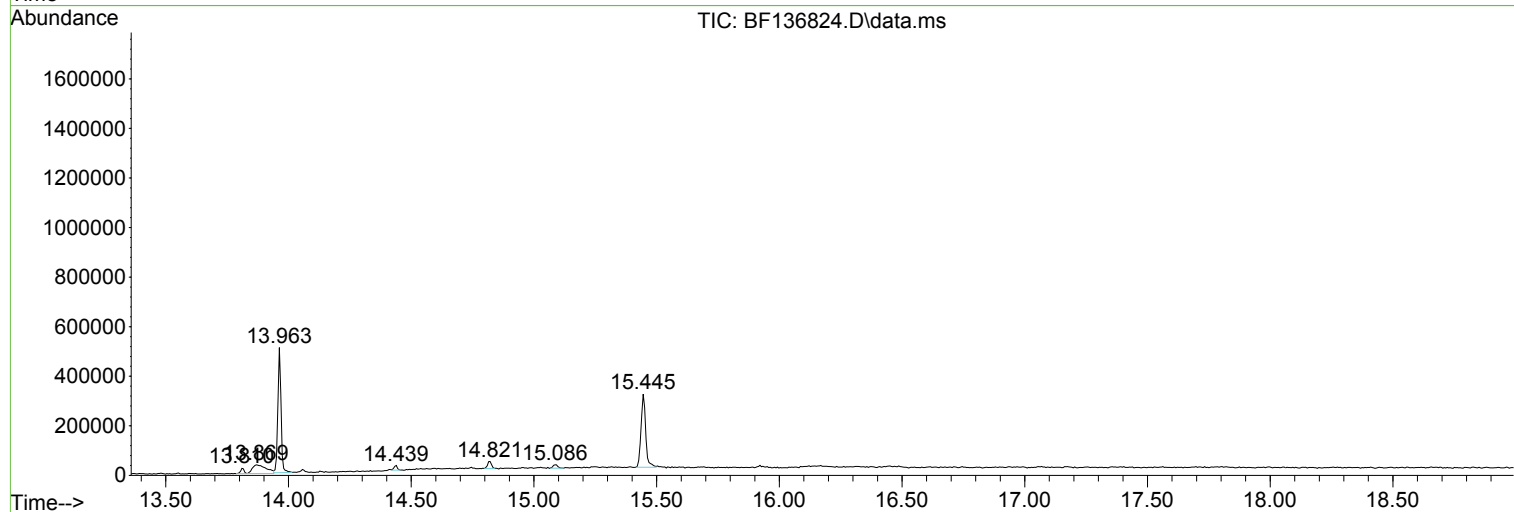
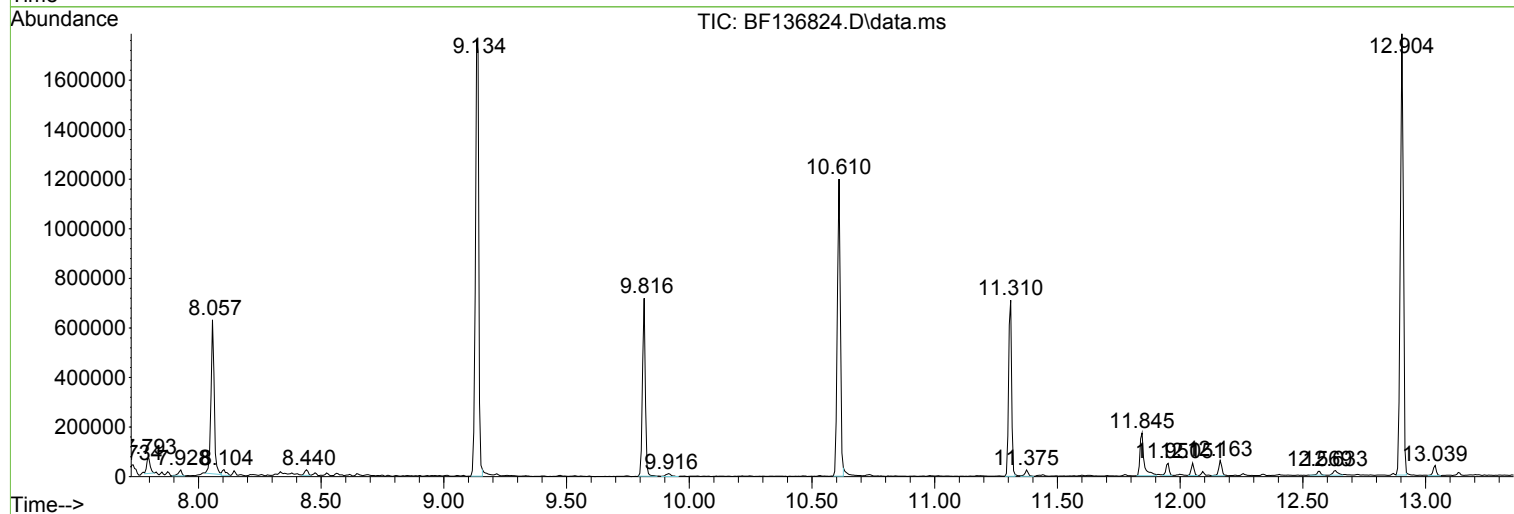
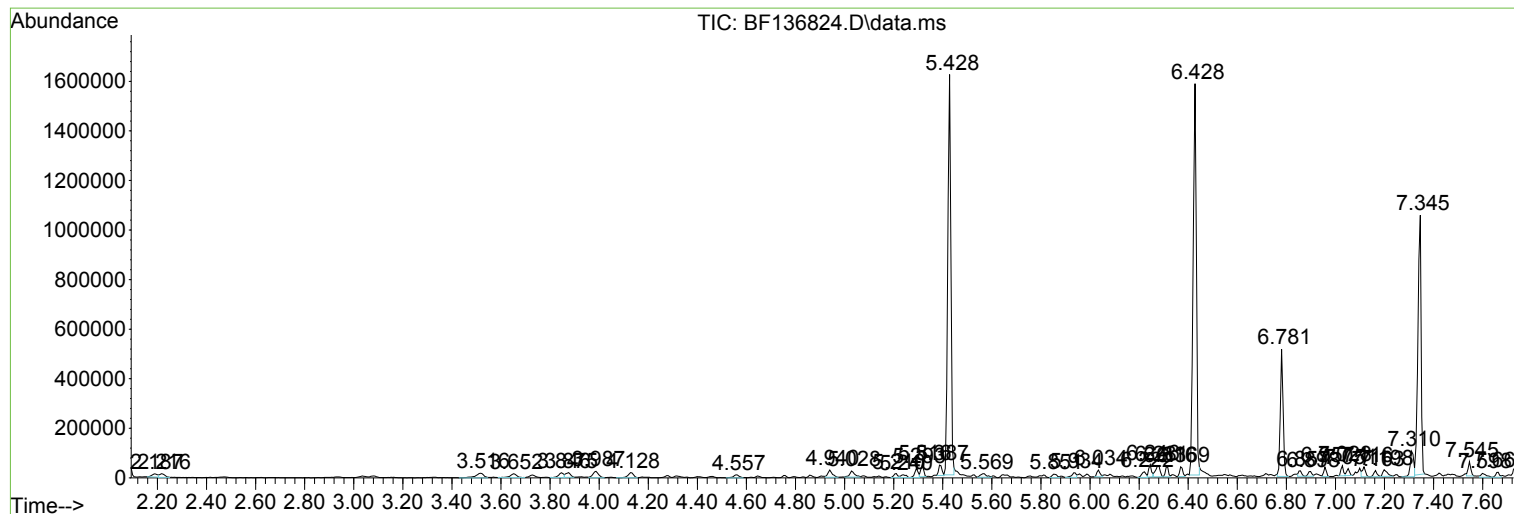
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB32-1-20231222-10.0-11.0

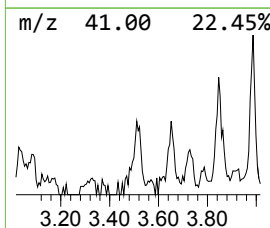
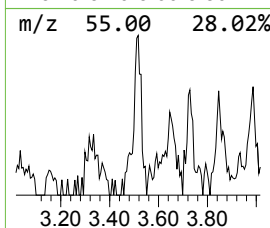
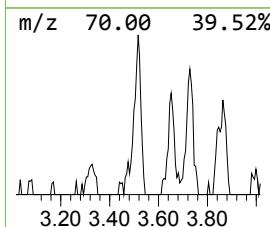
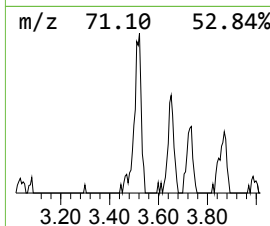
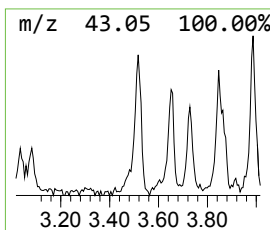
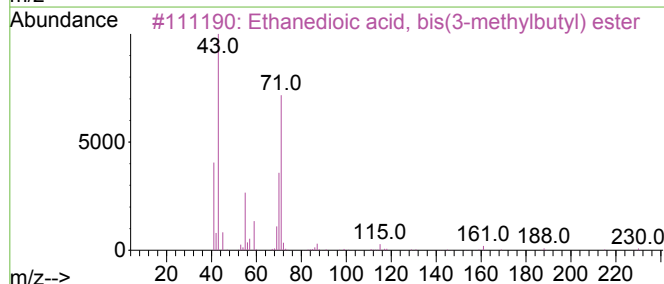
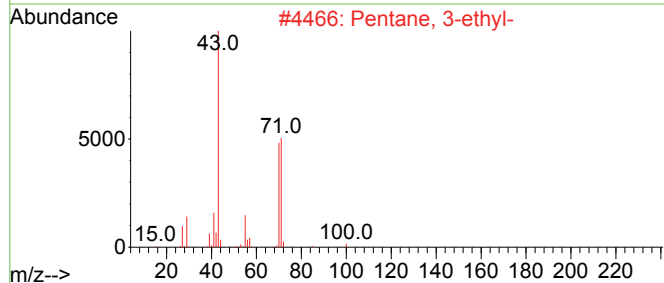
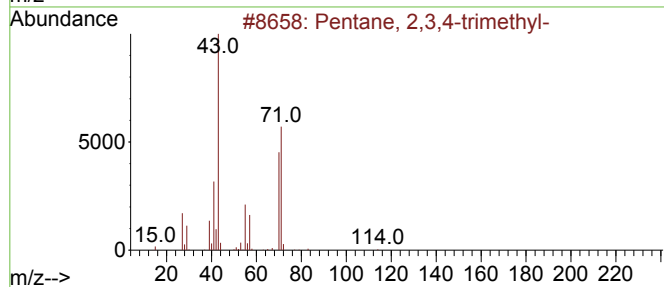
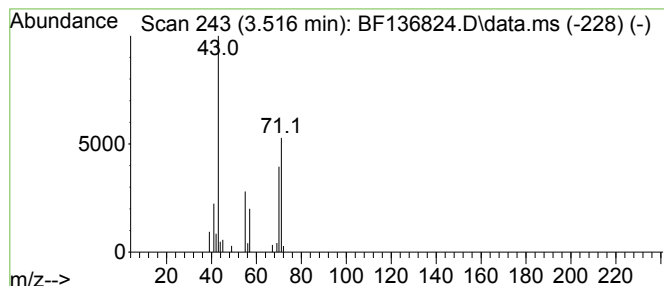
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	2.12 ng	42869	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	72
3			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64
4			Pentane, 2-nitro-	117	C5H11NO2	004609-89-6	47
5			Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	43



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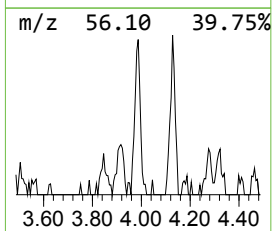
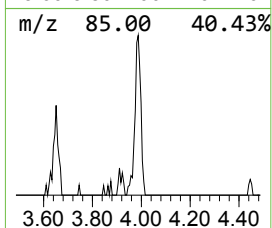
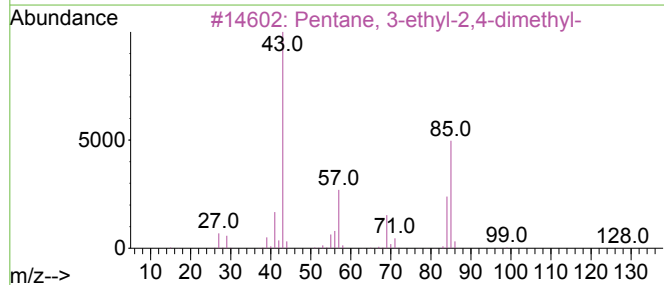
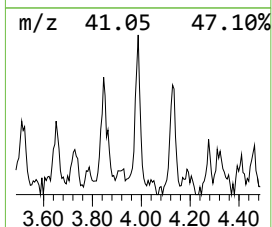
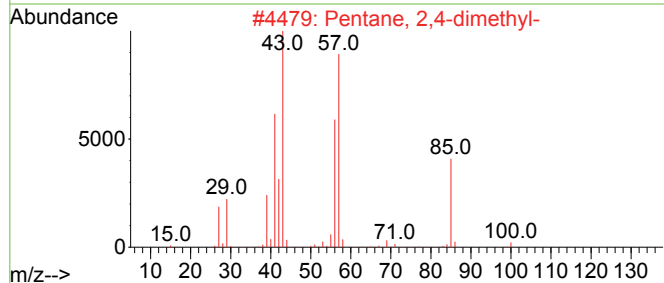
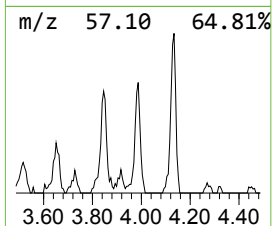
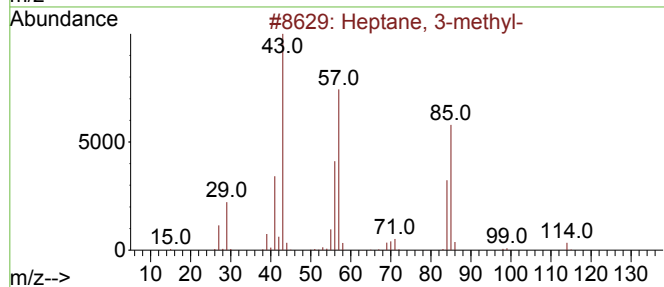
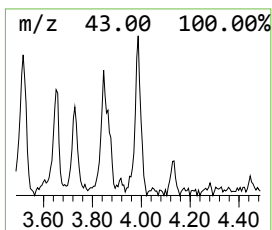
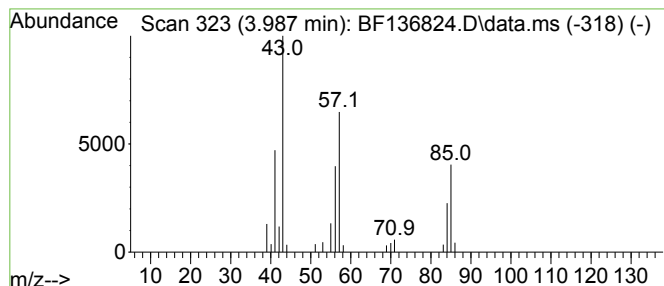
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Heptane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.987	2.01 ng	40774	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	78
2			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	53
3			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
4			Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	53
5			Hexane, 2-methyl-	100	C7H16	000591-76-4	50



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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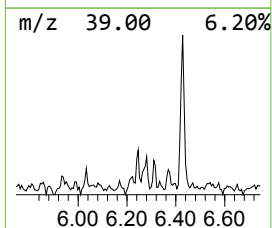
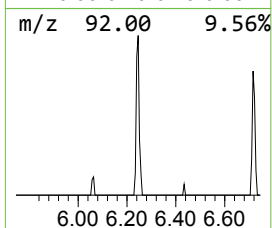
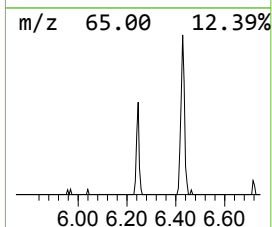
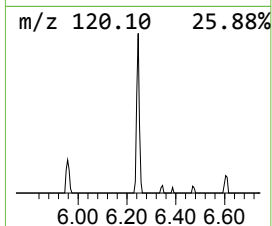
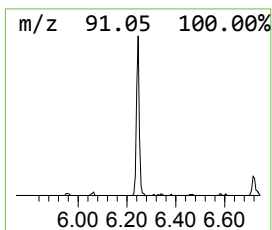
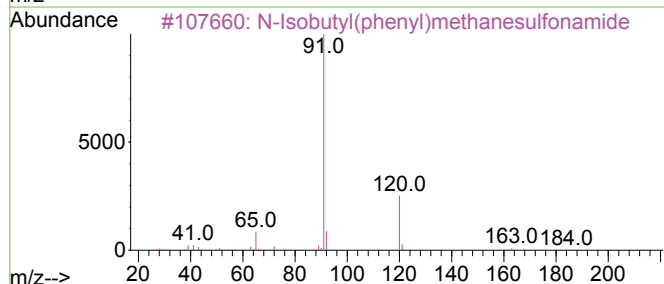
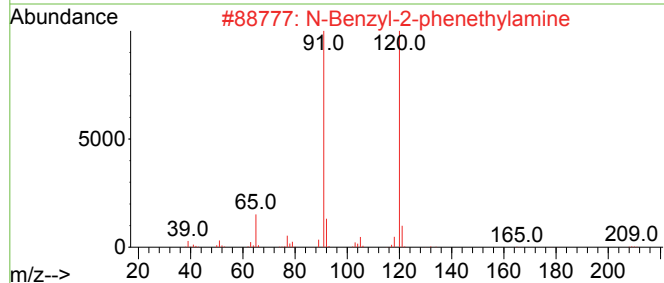
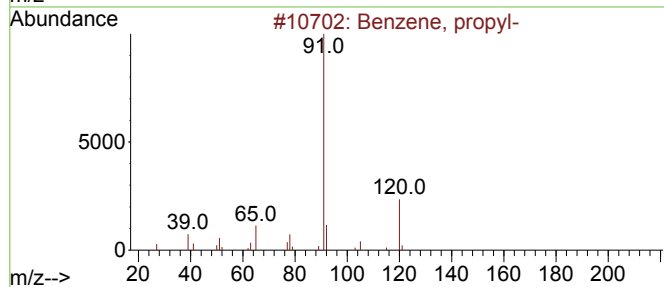
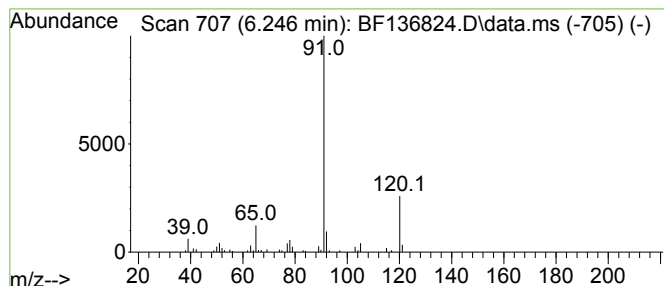
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.246	2.02 ng	40955	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	90
2			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	78
3			N-Isobutyl(phenyl)methanesulfona...	227	C11H17NO2S	144615-94-1	72
4			1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	64
5			N-Butylbenzylamine	163	C11H17N	002403-22-7	64



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Instrument :
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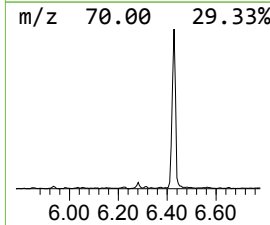
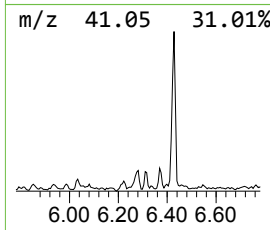
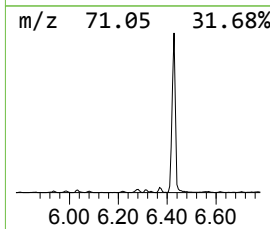
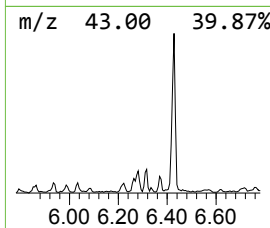
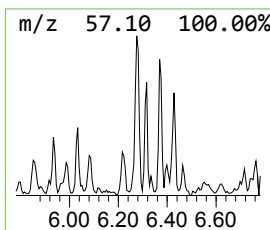
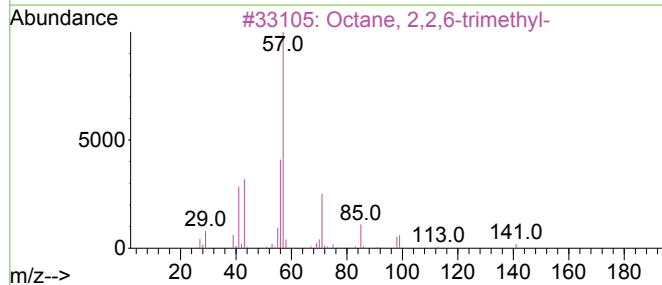
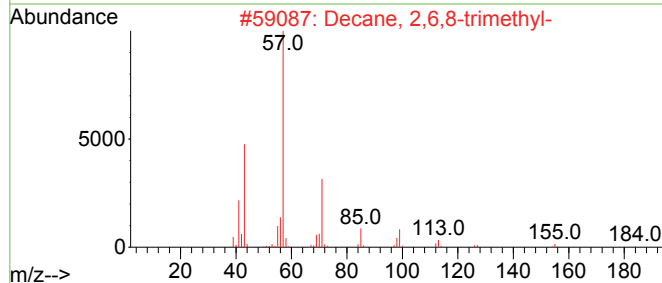
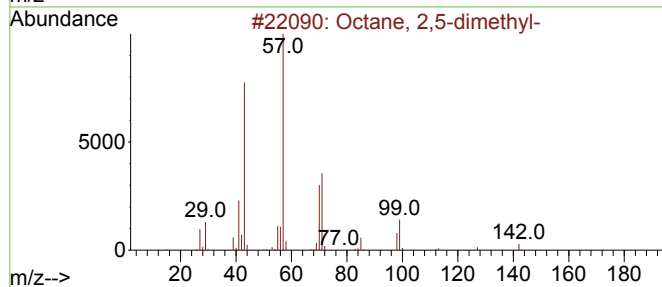
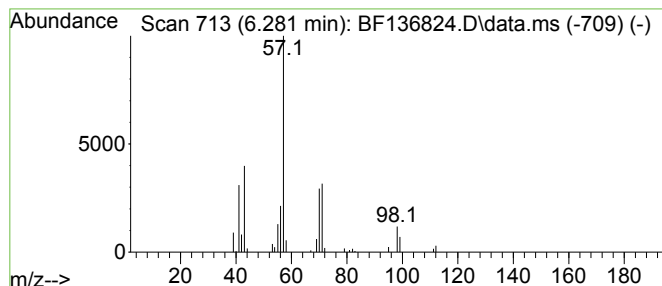
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octane, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.281	2.82 ng	56991	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	53
2			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	50
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	47
4			Nonane, 4-methyl-	142	C10H22	017301-94-9	45
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
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Acq On : 29 Dec 2023 12:36
Operator : CG\JU
Sample : 06017-06
Misc :
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Instrument :
BNA_F
ClientSampleId :
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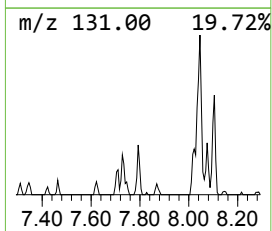
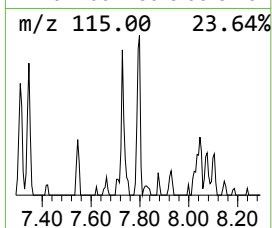
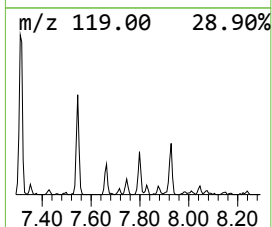
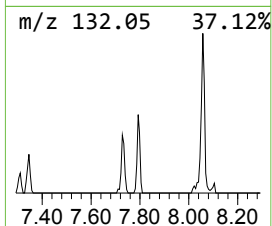
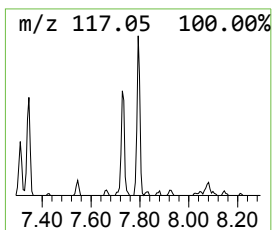
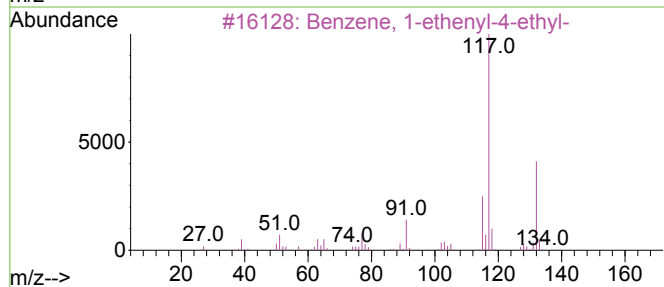
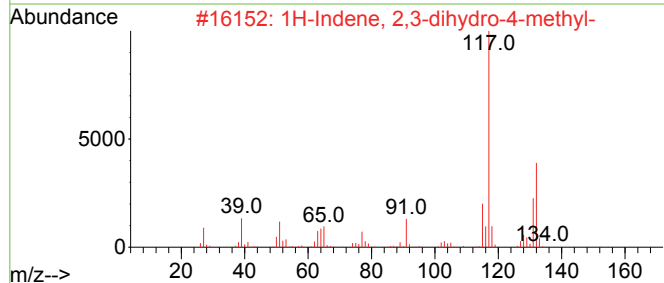
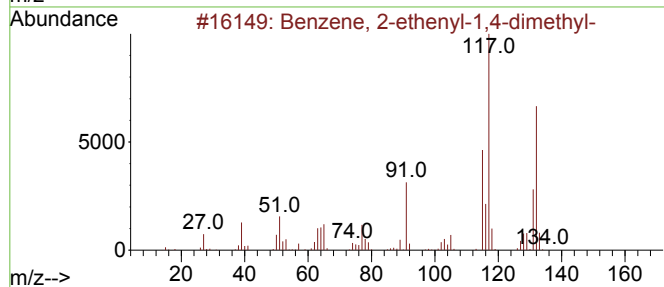
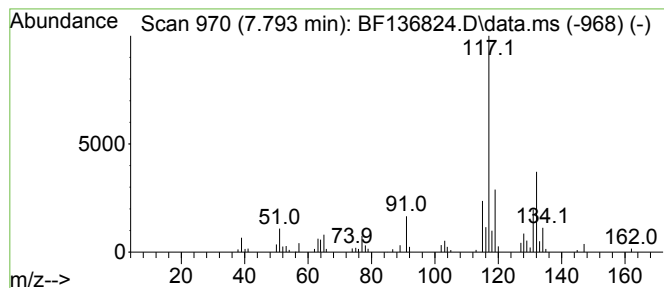
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.793	2.23 ng	63423	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	92
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136824.D
Acq On : 29 Dec 2023 12:36
Operator : CG\JU
Sample : 06017-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB32-1-20231222-10.0-11.0

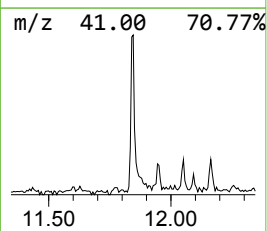
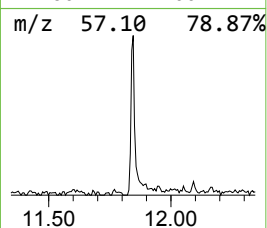
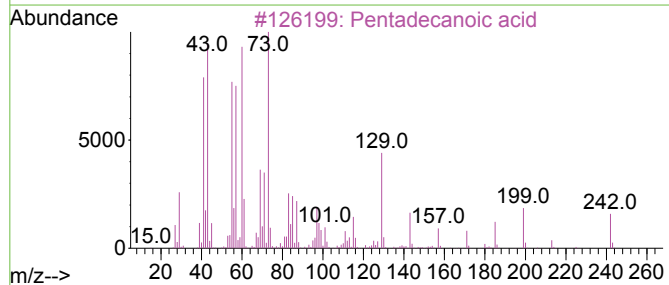
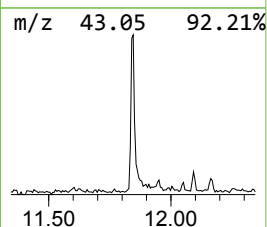
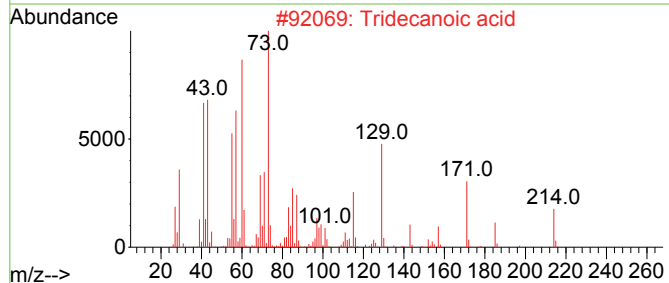
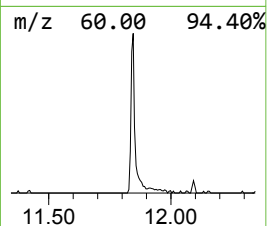
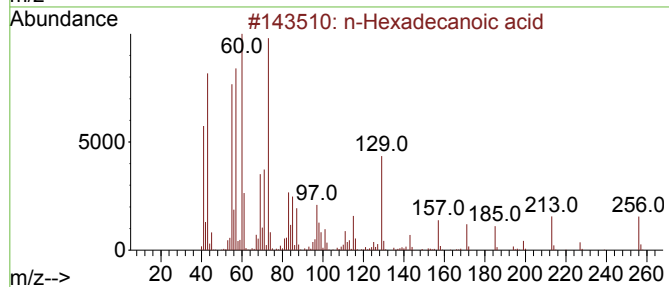
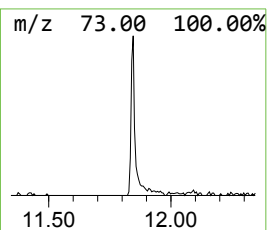
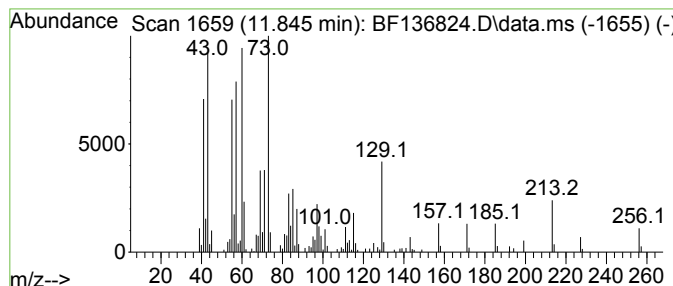
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	6.50 ng	197653	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	96
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136824.D
Acq On : 29 Dec 2023 12:36
Operator : CG\JU
Sample : 06017-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB32-1-20231222-10.0-11.0

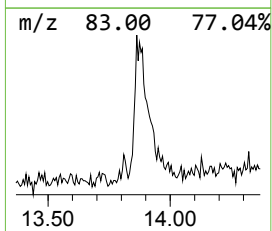
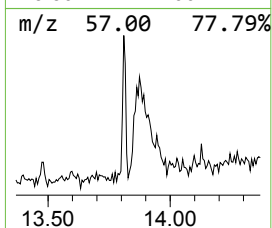
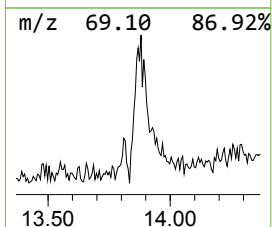
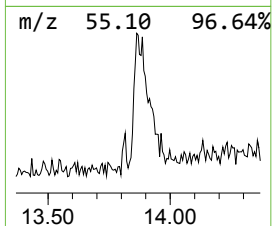
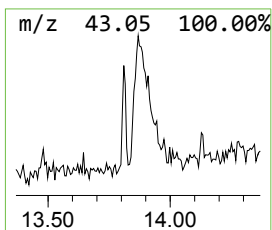
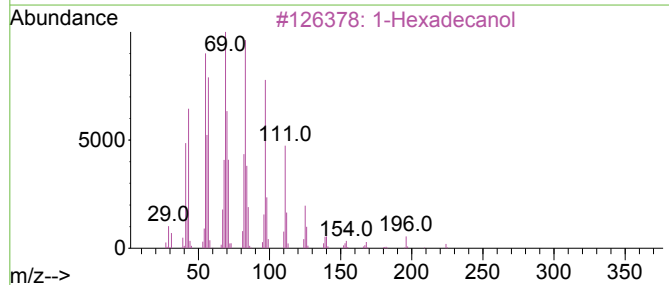
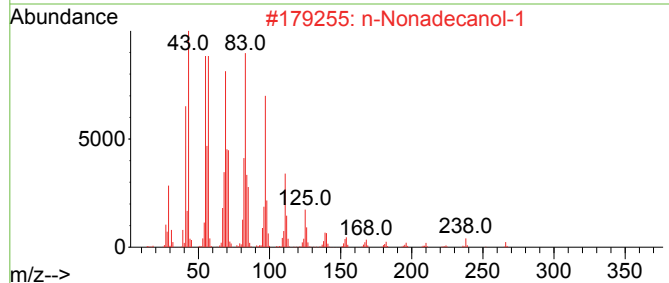
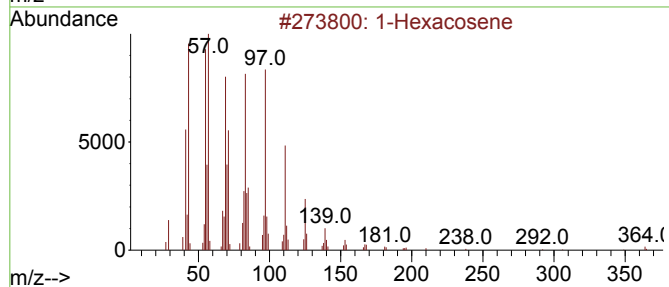
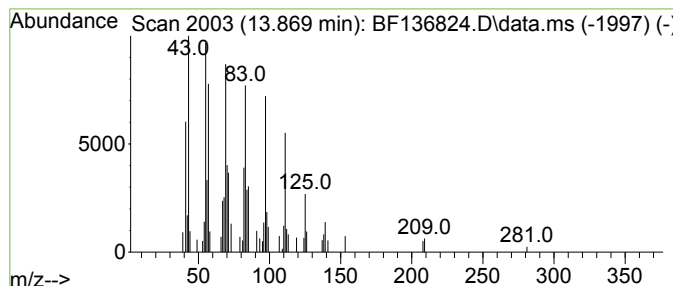
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.869	5.97 ng	135587	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	93
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3			1-Hexadecanol	242	C16H34O	036653-82-4	87
4			1-Tetracosene	336	C24H48	010192-32-2	87
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136824.D
Acq On : 29 Dec 2023 12:36
Operator : CG\JU
Sample : 06017-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB32-1-20231222-10.0-11.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
Pentane, 2,3,4-...	3.516	2.1	ng	42869	1	6.781	404733	20.0
Heptane, 3-methyl-	3.987	2.0	ng	40774	1	6.781	404733	20.0
Benzene, propyl-	6.246	2.0	ng	40955	1	6.781	404733	20.0
Octane, 2,5-dim...	6.281	2.8	ng	56991	1	6.781	404733	20.0
Benzene, 2-ethe...	7.793	2.2	ng	63423	2	8.057	567956	20.0
n-Hexadecanoic ...	11.845	6.5	ng	197653	4	11.310	608154	20.0
1-Hexacosene	13.869	6.0	ng	135587	5	13.963	454202	20.0