

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
 Data File : BF138991.D
 Acq On : 14 Aug 2024 13:37
 Operator : RC/JU
 Sample : P3474-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-A1-COMP

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138991.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	16	21	29	rVB	6691	11369	1.32%	0.190%
2	3.446	223	230	240	rBV3	2172	9057	1.05%	0.152%
3	5.057	498	504	522	rVB	45072	72166	8.38%	1.208%
4	5.469	569	574	597	rBV	523988	740670	85.98%	12.394%
5	6.481	741	746	770	rBV	577499	783885	90.99%	13.117%
6	6.834	802	806	813	rVB	208206	253620	29.44%	4.244%
7	7.398	897	902	918	rBV	384547	502585	58.34%	8.410%
8	8.116	1019	1024	1039	rBV	269593	334072	38.78%	5.590%
9	8.439	1074	1079	1089	rBV	12662	22380	2.60%	0.375%
10	9.186	1201	1206	1211	rBV	713568	861478	100.00%	14.416%
11	9.869	1317	1322	1327	rBV	290887	363124	42.15%	6.076%
12	9.957	1332	1337	1344	rBV	11053	17440	2.02%	0.292%
13	10.657	1451	1456	1470	rBV	335375	433082	50.27%	7.247%
14	11.357	1570	1575	1589	rVB	240147	311704	36.18%	5.216%
15	11.874	1658	1663	1677	rBV2	16905	31390	3.64%	0.525%
16	12.933	1838	1843	1848	rBV	470420	571425	66.33%	9.562%
17	13.145	1872	1879	1885	rBV3	6444	13019	1.51%	0.218%
18	13.751	1976	1982	1989	rBV	8505	14291	1.66%	0.239%
19	13.857	1996	2000	2013	rVB6	8491	24469	2.84%	0.409%
20	13.998	2019	2024	2032	rVB	155719	202278	23.48%	3.385%
21	14.139	2043	2048	2056	rVB	8660	11863	1.38%	0.199%
22	14.257	2062	2068	2078	rBV2	9587	17856	2.07%	0.299%
23	14.439	2093	2099	2105	rBV	15398	22791	2.65%	0.381%
24	14.710	2139	2145	2147	rBV2	6910	10966	1.27%	0.184%
25	14.745	2147	2151	2155	rVV	16701	24105	2.80%	0.403%
26	14.815	2159	2163	2168	rVB	13246	17686	2.05%	0.296%
27	15.074	2201	2207	2214	rVB	18643	29063	3.37%	0.486%
28	15.186	2219	2226	2234	rBV6	4997	12504	1.45%	0.209%
29	15.462	2264	2273	2285	rBV	115965	199827	23.20%	3.344%
30	15.874	2337	2343	2349	rBV	12968	21663	2.51%	0.363%
31	16.368	2419	2427	2436	rVB2	10001	23965	2.78%	0.401%
32	16.945	2519	2525	2532	rVB4	4434	10126	1.18%	0.169%

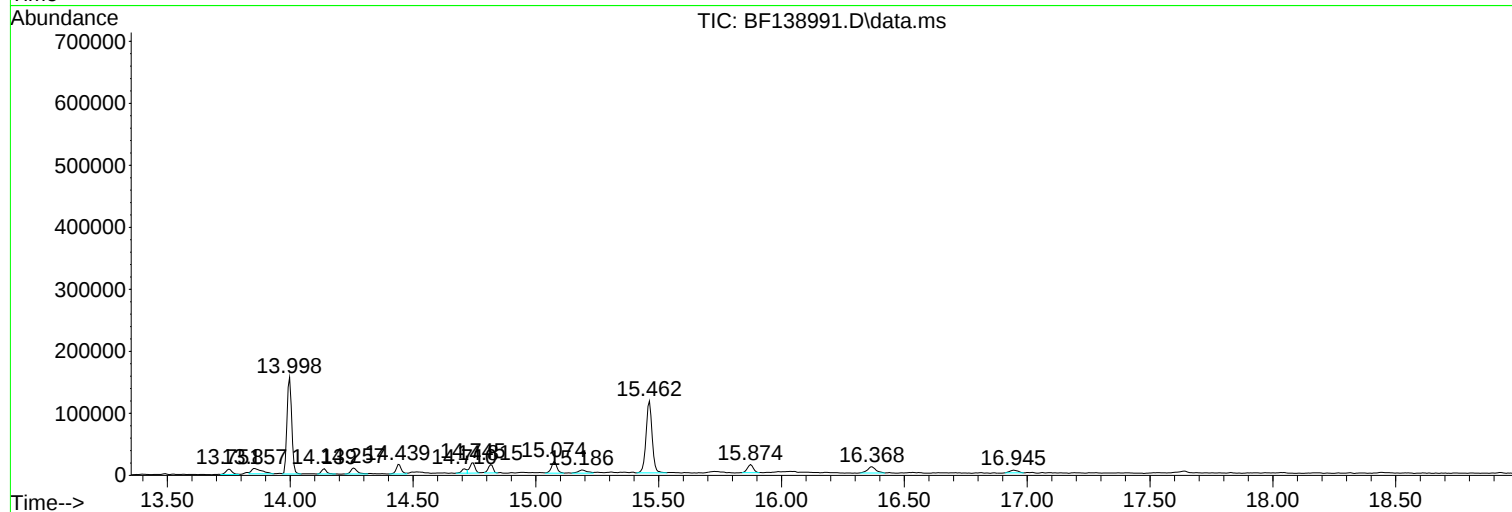
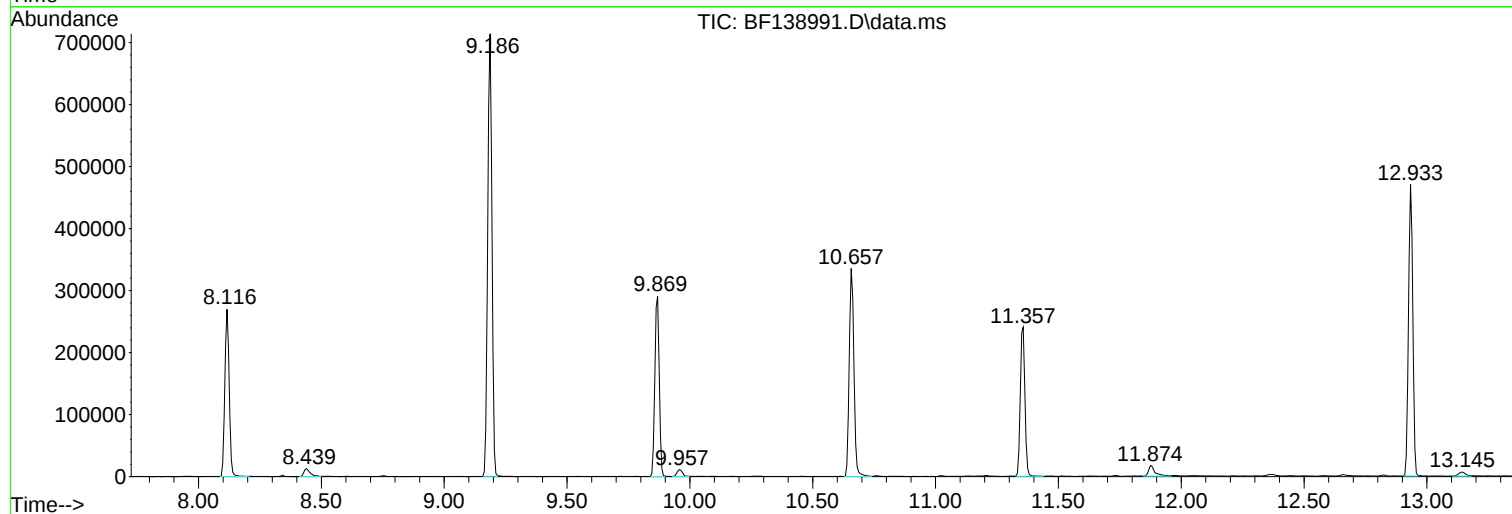
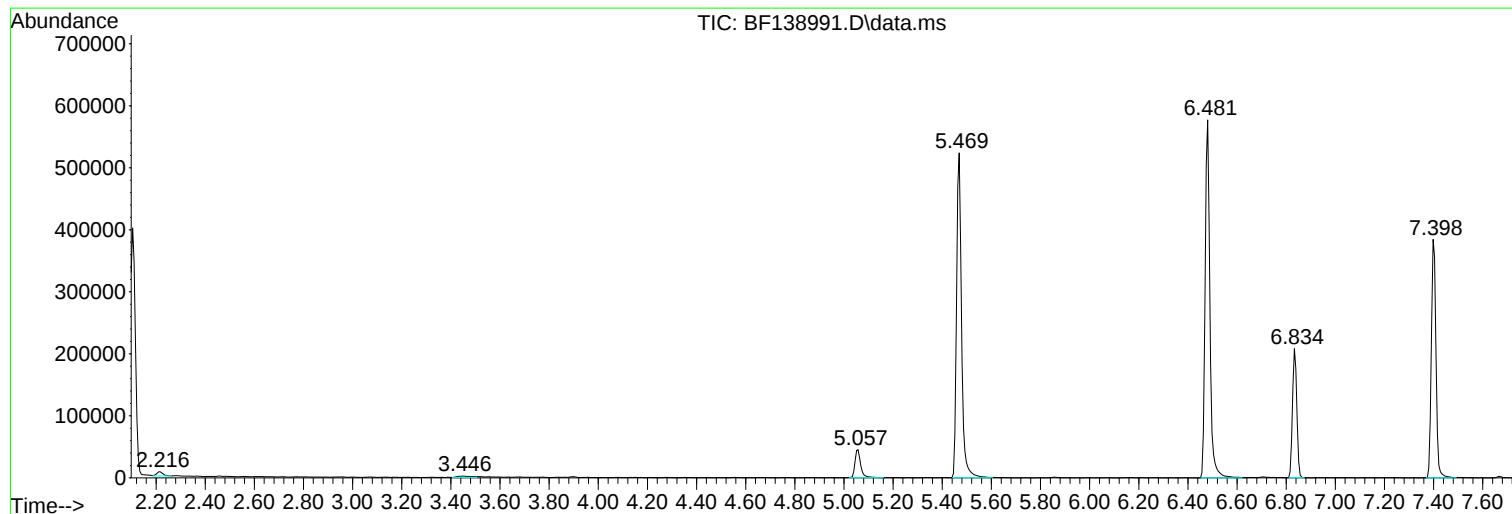
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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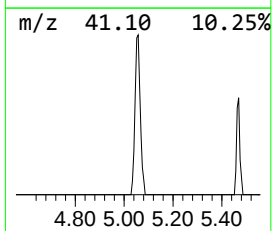
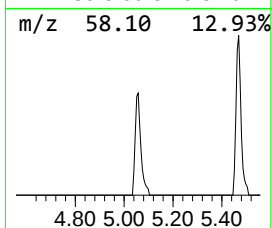
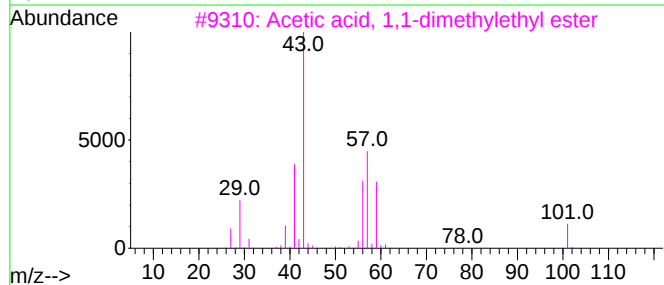
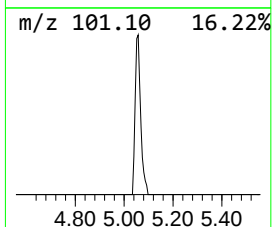
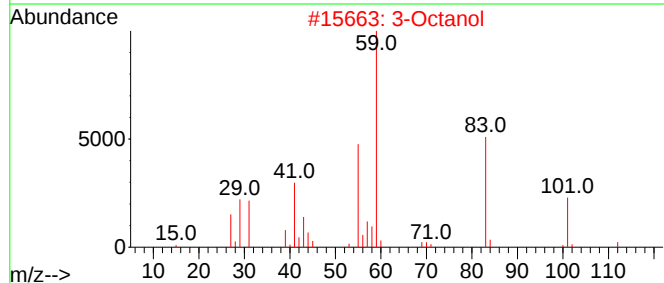
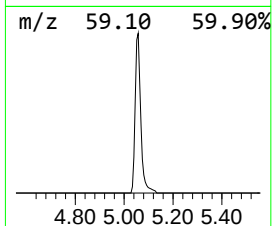
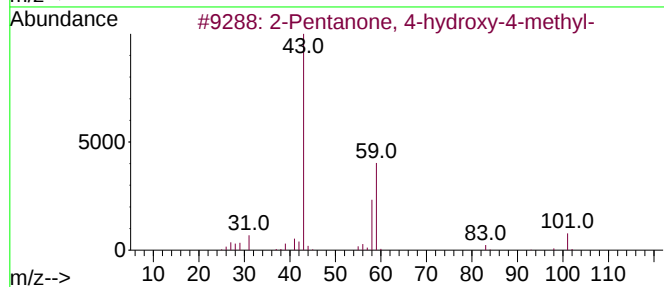
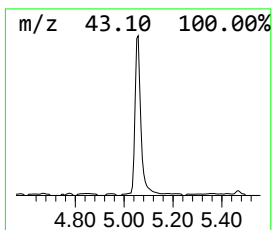
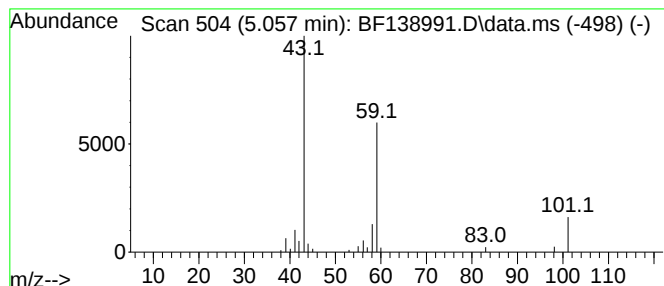
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	5.69 ng	72166	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16		



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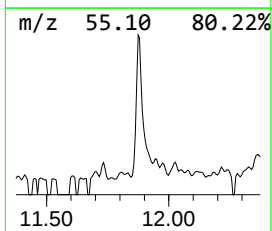
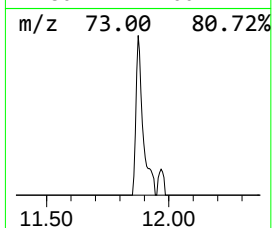
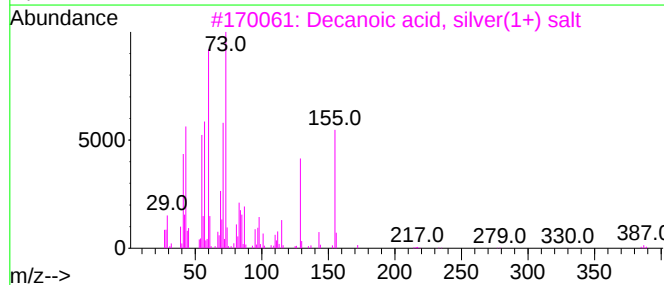
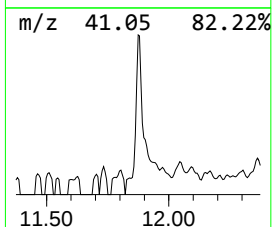
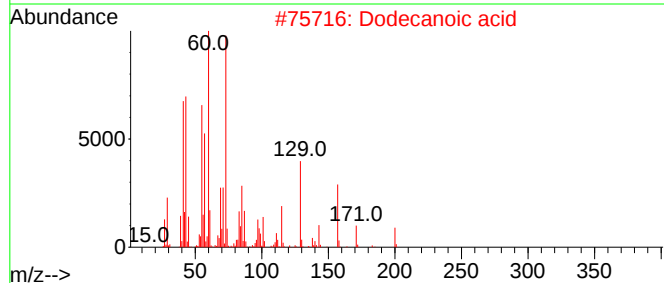
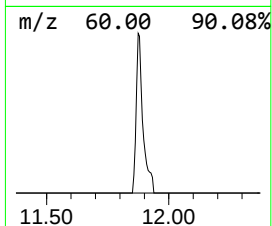
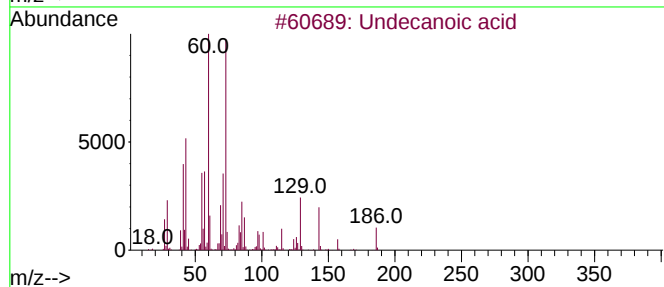
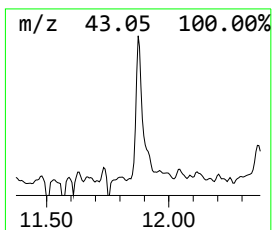
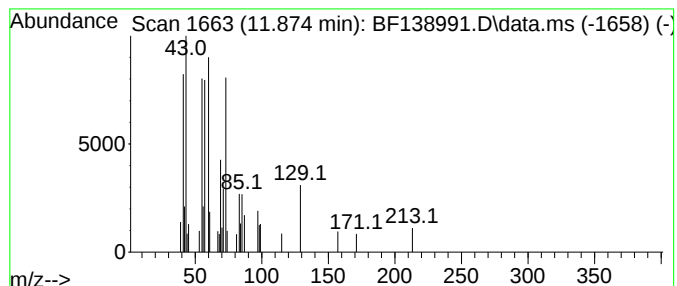
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Peak Number 2 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	2.01 ng	31390	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	64
2			Dodecanoic acid	200	C12H24O2	000143-07-7	59
3			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	47



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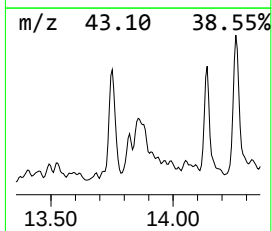
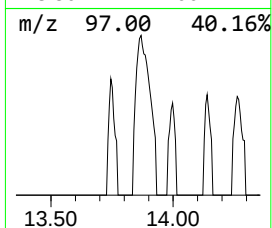
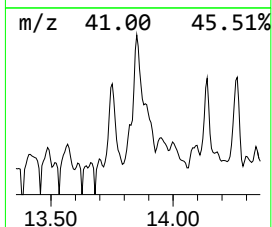
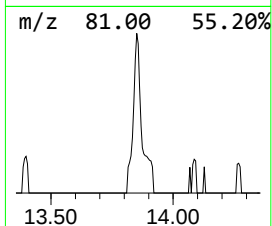
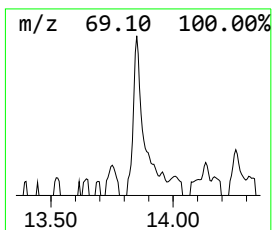
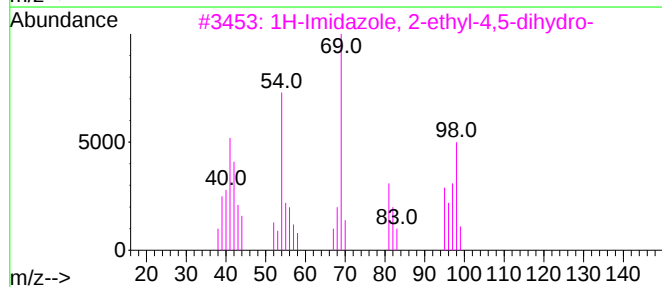
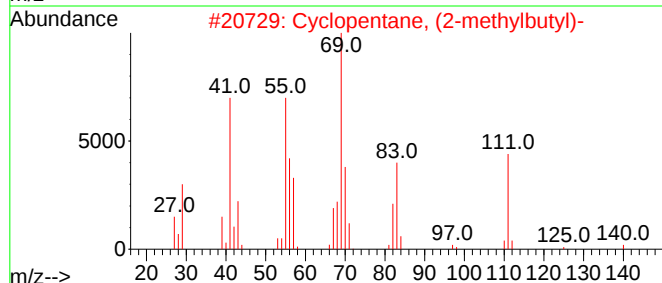
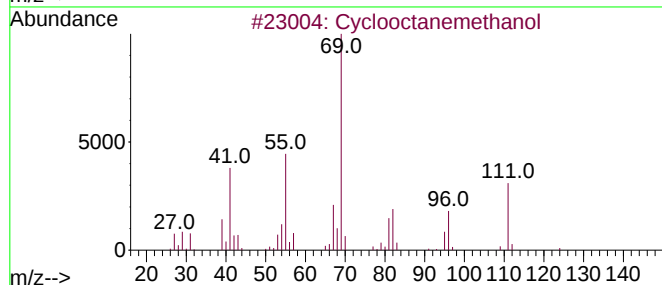
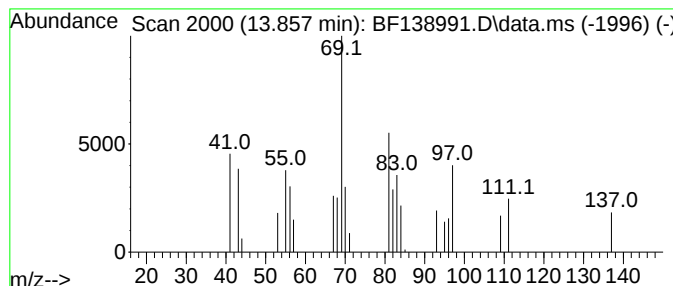
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Peak Number 3 unknown13.857 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.42 ng	24469	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctanemethanol	142	C9H18O	003637-63-6	38
2			Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	38
3			1H-Imidazole, 2-ethyl-4,5-dihydro-	98	C5H10N2	000930-52-9	37
4			Geranyl bromide	216	C10H17Br	006138-90-5	35
5			Cyclopentaneethanol, .beta.,2,3-...	156	C10H20O	021721-18-6	33



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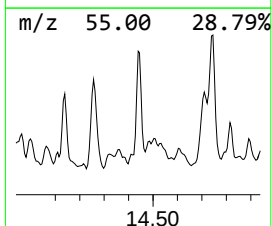
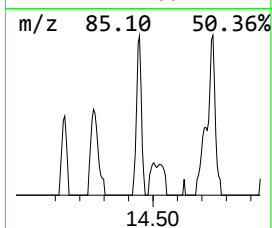
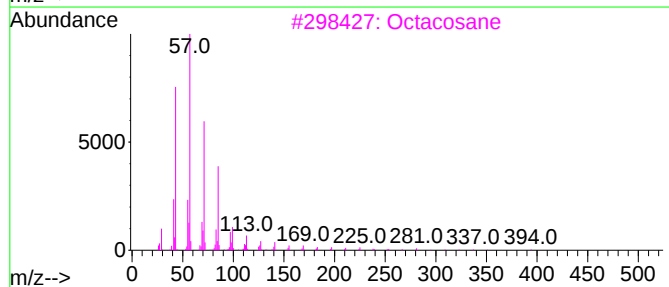
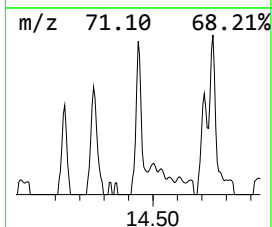
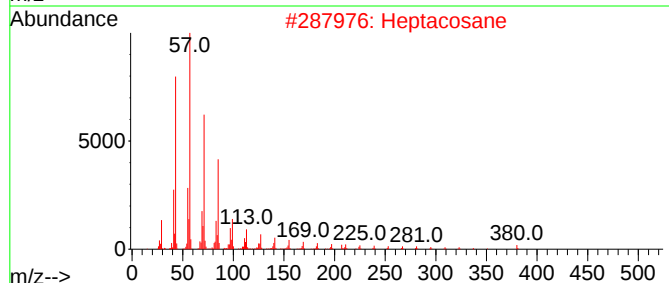
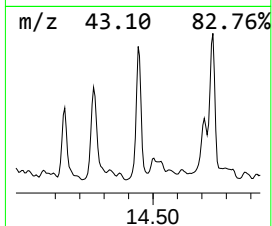
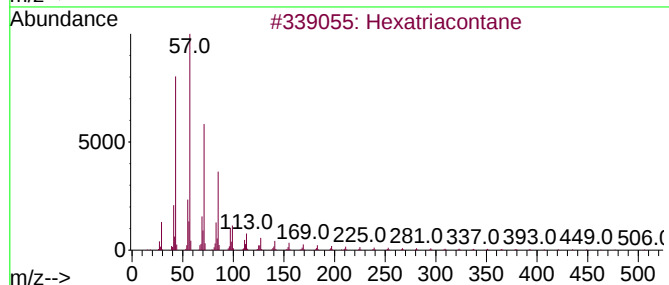
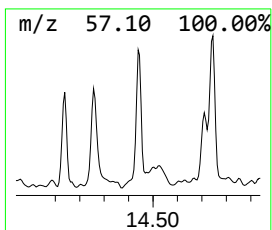
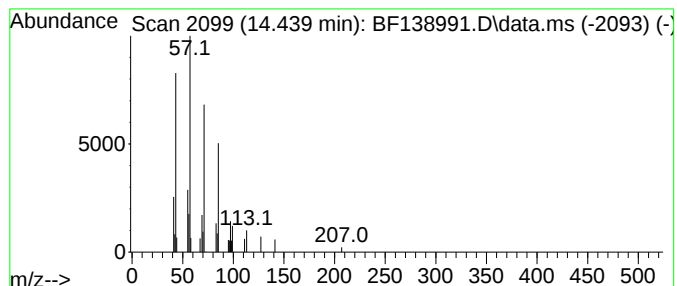
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Peak Number 4 Hexatriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	2.25 ng	22791	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			10-Methylnonadecane	282	C20H42	056862-62-5	91
5			Tetratetracontane	619	C44H90	007098-22-8	91



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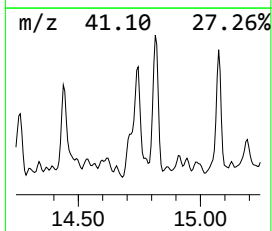
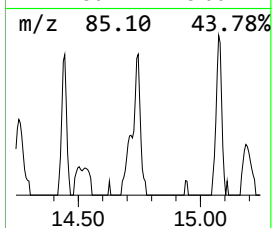
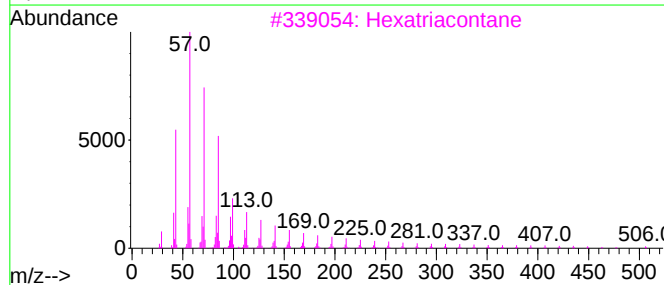
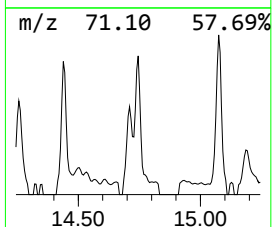
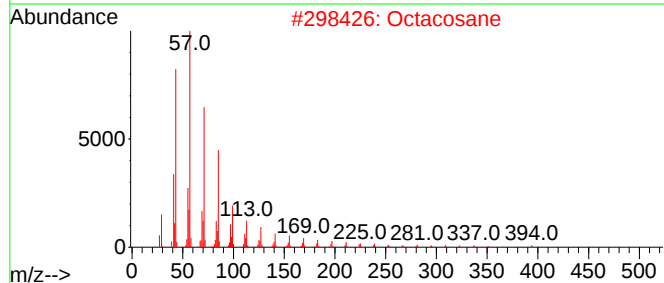
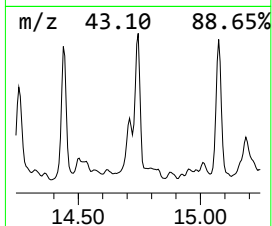
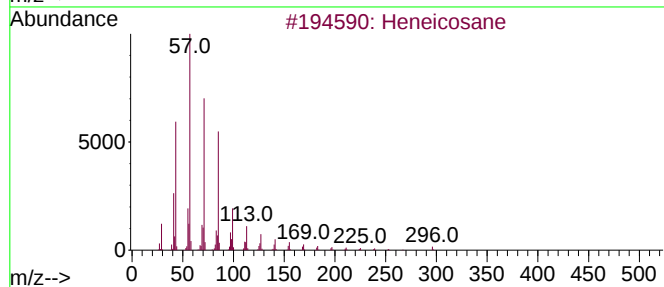
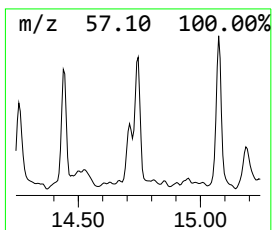
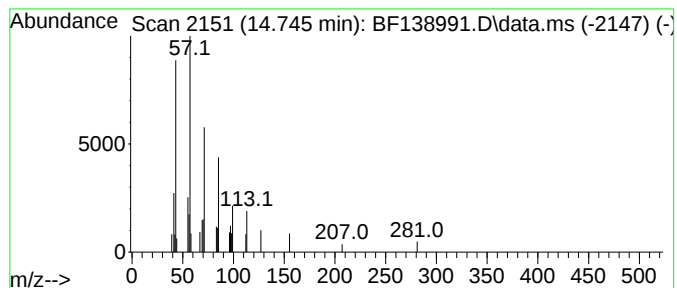
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Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.41 ng	24105	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	86
2			Octacosane	394	C28H58	000630-02-4	80
3			Hexatriacontane	507	C36H74	000630-06-8	72
4			Pentacosane	352	C25H52	000629-99-2	64
5			10-Methylnonadecane	282	C20H42	056862-62-5	64



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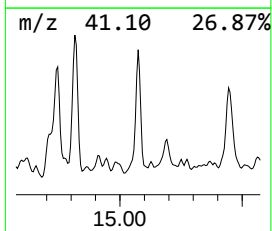
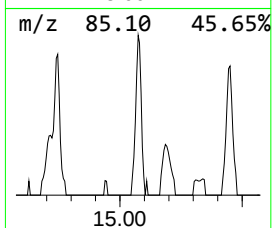
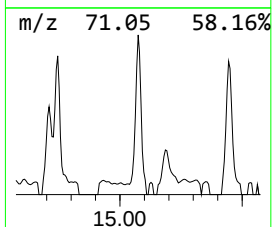
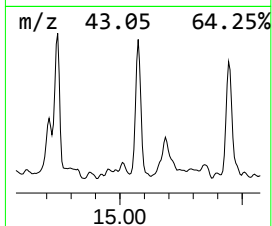
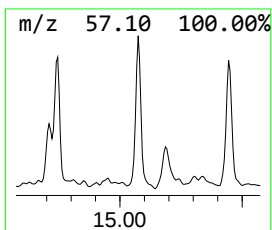
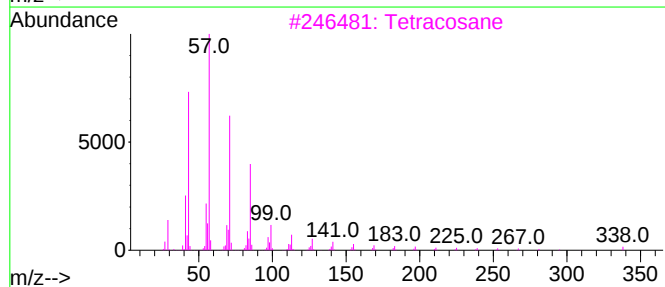
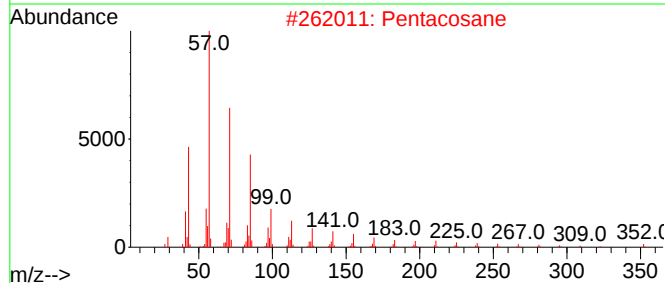
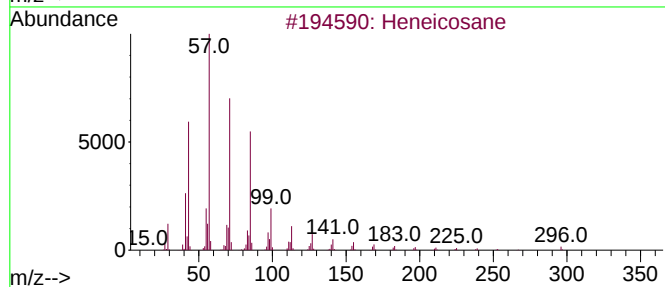
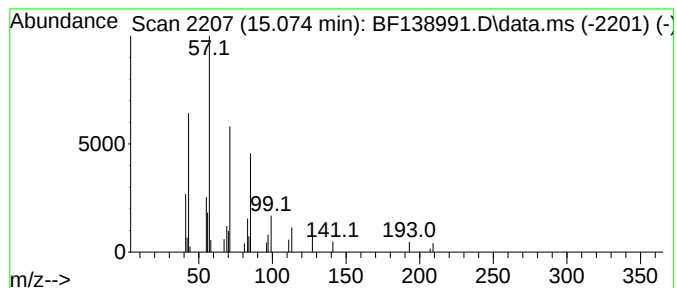
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	2.91 ng	29063	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	86
2			Pentacosane	352	C25H52	000629-99-2	86
3			Tetracosane	338	C24H50	000646-31-1	86
4			Hexacosane	366	C26H54	000630-01-3	86
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138991.D
Acq On : 14 Aug 2024 13:37
Operator : RC/JU
Sample : P3474-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-A1-COMP

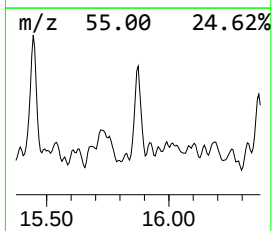
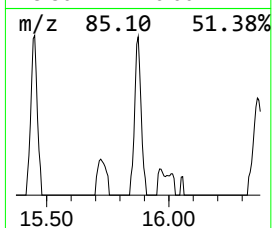
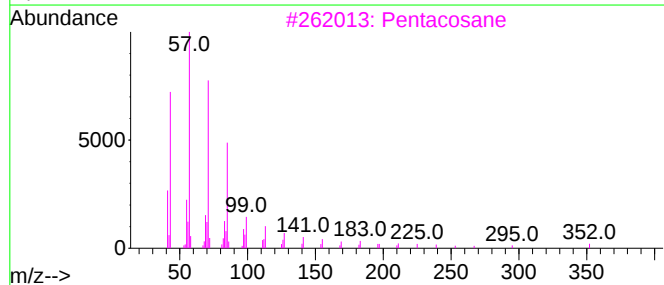
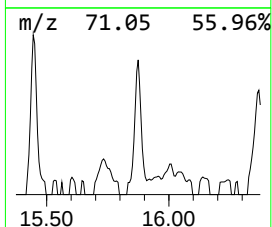
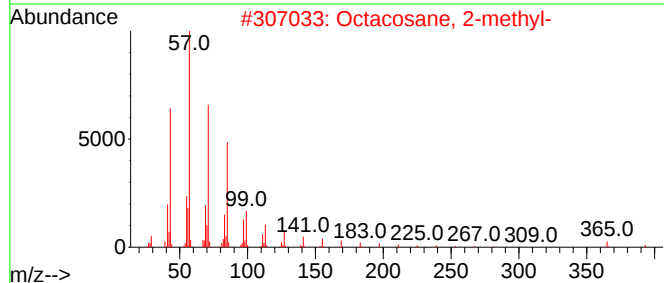
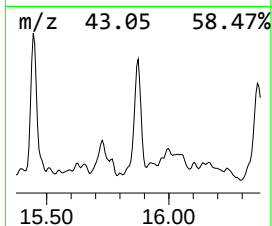
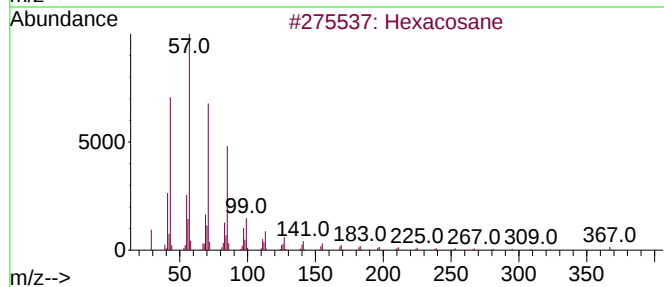
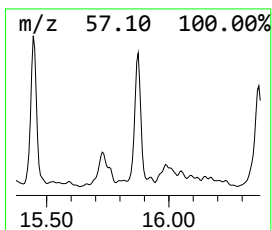
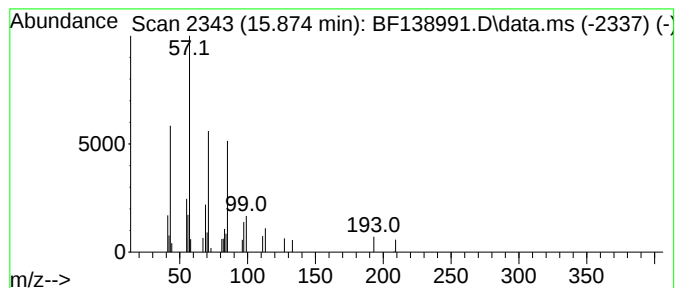
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	2.17 ng	21663	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	86
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
3			Pentacosane	352	C25H52	000629-99-2	78
4			Tetratetracontane	619	C44H90	007098-22-8	78
5			Heneicosane	296	C21H44	000629-94-7	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138991.D
Acq On : 14 Aug 2024 13:37
Operator : RC/JU
Sample : P3474-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

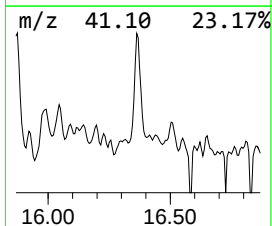
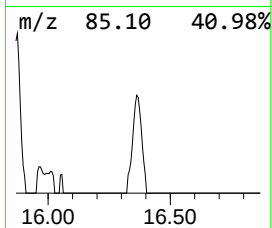
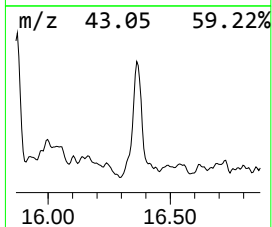
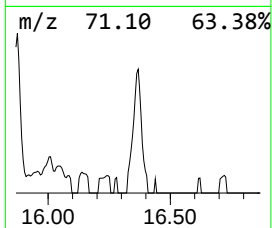
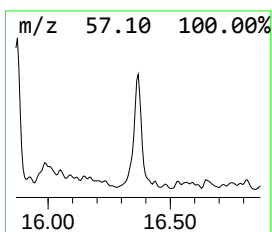
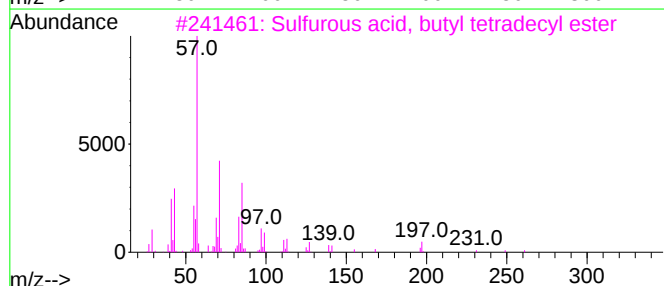
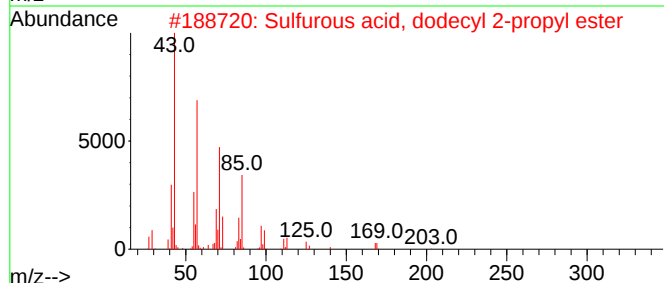
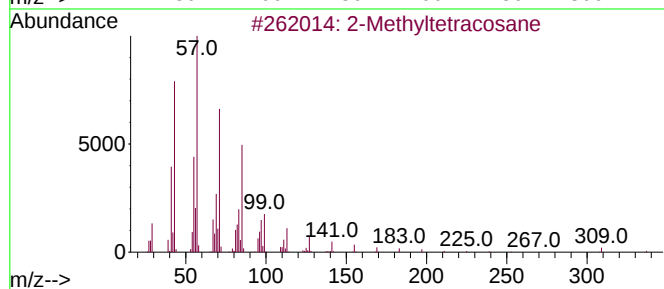
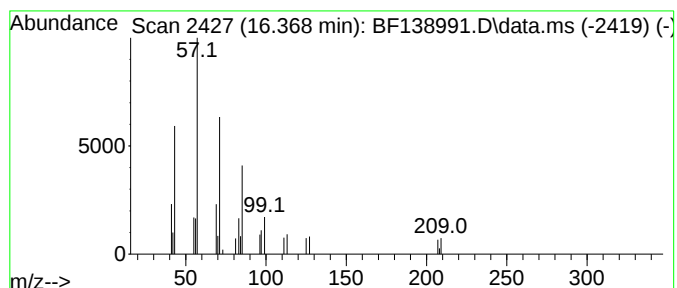
Instrument :
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ClientSampleId :
WC-A1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Methyltetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.368	2.40 ng	23965	Perylene-d12	15.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyltetracosane	352	C25H52	001560-78-7	87
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80
3	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	80
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
5	Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081424\
Data File : BF138991.D
Acq On : 14 Aug 2024 13:37
Operator : RC/JU
Sample : P3474-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-A1-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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-...	5.057	5.7	ng	72166	1	6.834	253620	20.0
Undecanoic acid	11.874	2.0	ng	31390	4	11.357	311704	20.0
unknown13.857	13.857	2.4	ng	24469	5	13.998	202278	20.0
Hexatriacontane	14.439	2.3	ng	22791	5	13.998	202278	20.0
Heneicosane	14.745	2.4	ng	24105	6	15.462	199827	20.0
Pentacosane	15.074	2.9	ng	29063	6	15.462	199827	20.0
Hexacosane	15.874	2.2	ng	21663	6	15.462	199827	20.0
2-Methyltetraco...	16.368	2.4	ng	23965	6	15.462	199827	20.0