

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136744.D
 Acq On : 27 Dec 2023 04:17
 Operator : CG\JU
 Sample : 05602-11
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROUTE-4-TP-6

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: BF136744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	18	rVB3	13438	20053	1.85%	0.226%
2	3.851	297	300	306	rVB	12061	15797	1.46%	0.178%
3	5.010	494	497	506	rVB	34714	41913	3.86%	0.472%
4	5.422	563	567	582	rBV	1167559	1084540	100.00%	12.213%
5	6.428	734	738	741	rBV	1154816	1018949	93.95%	11.474%
6	6.781	795	798	802	rBV	449645	374435	34.52%	4.217%
7	7.345	889	894	897	rBV	756438	645009	59.47%	7.264%
8	8.057	1012	1015	1019	rBV	507779	415714	38.33%	4.681%
9	9.133	1195	1198	1202	rBV	1171367	1042888	96.16%	11.744%
10	9.257	1215	1219	1223	rBV	170011	155846	14.37%	1.755%
11	9.816	1311	1314	1317	rBV	505330	374811	34.56%	4.221%
12	10.610	1445	1449	1459	rVB	607403	524928	48.40%	5.911%
13	10.727	1466	1469	1473	rVB3	18367	26553	2.45%	0.299%
14	11.310	1564	1568	1571	rBV	427733	384270	35.43%	4.327%
15	11.363	1574	1577	1583	rVB5	9415	15272	1.41%	0.172%
16	11.774	1644	1647	1651	rBV5	9283	11865	1.09%	0.134%
17	11.845	1655	1659	1670	rVV2	177729	203993	18.81%	2.297%
18	12.363	1744	1747	1750	rBV5	16002	20508	1.89%	0.231%
19	12.527	1770	1775	1777	rBV	50066	52356	4.83%	0.590%
20	12.569	1779	1782	1788	rVB3	28488	35450	3.27%	0.399%
21	12.633	1790	1793	1797	rBV2	49900	56229	5.18%	0.633%
22	12.692	1800	1803	1807	rVB4	13171	14054	1.30%	0.158%
23	12.757	1811	1814	1816	rVB	46065	35094	3.24%	0.395%
24	12.904	1835	1839	1842	rBV	1188794	1009906	93.12%	11.373%
25	13.092	1867	1871	1874	rVB	258111	251653	23.20%	2.834%
26	13.139	1876	1879	1881	rBV	15275	14775	1.36%	0.166%
27	13.810	1991	1993	1996	rBV	21361	19285	1.78%	0.217%
28	13.857	1996	2001	2013	rBV5	64903	200696	18.51%	2.260%
29	13.963	2015	2019	2022	rBV	409017	365529	33.70%	4.116%
30	14.439	2098	2100	2103	rVB	41329	35766	3.30%	0.403%
31	15.092	2209	2211	2219	rVB	98735	103469	9.54%	1.165%
32	15.445	2267	2271	2275	rBV	179818	219578	20.25%	2.473%
33	15.933	2350	2354	2358	rVB	65940	88954	8.20%	1.002%

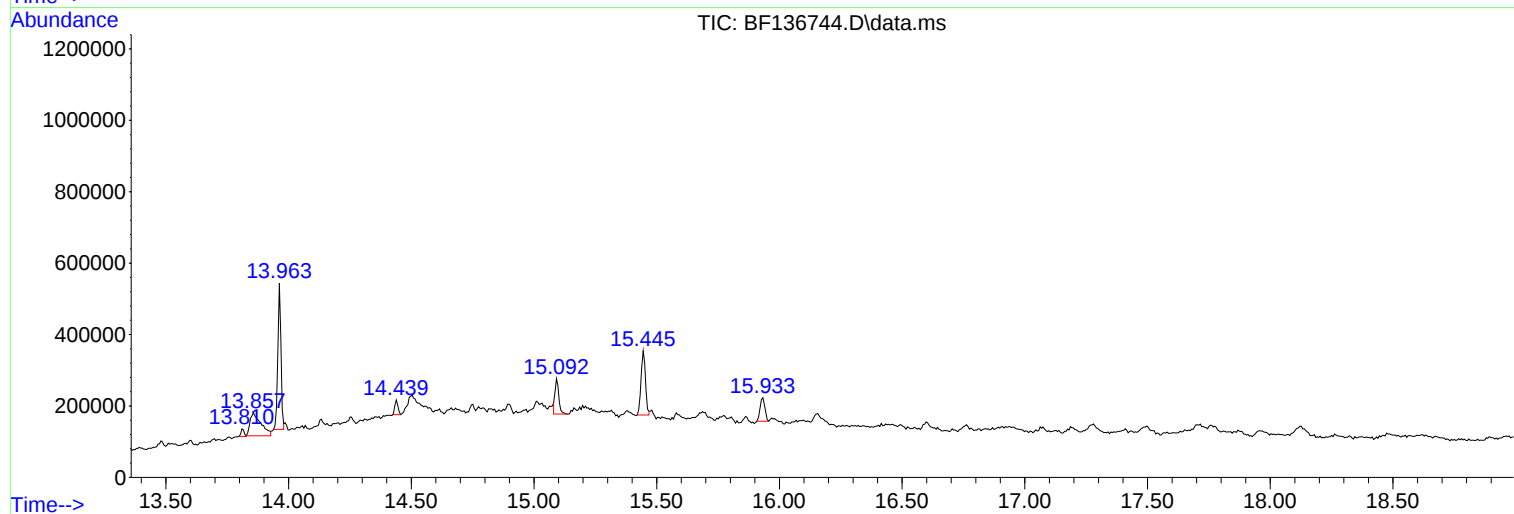
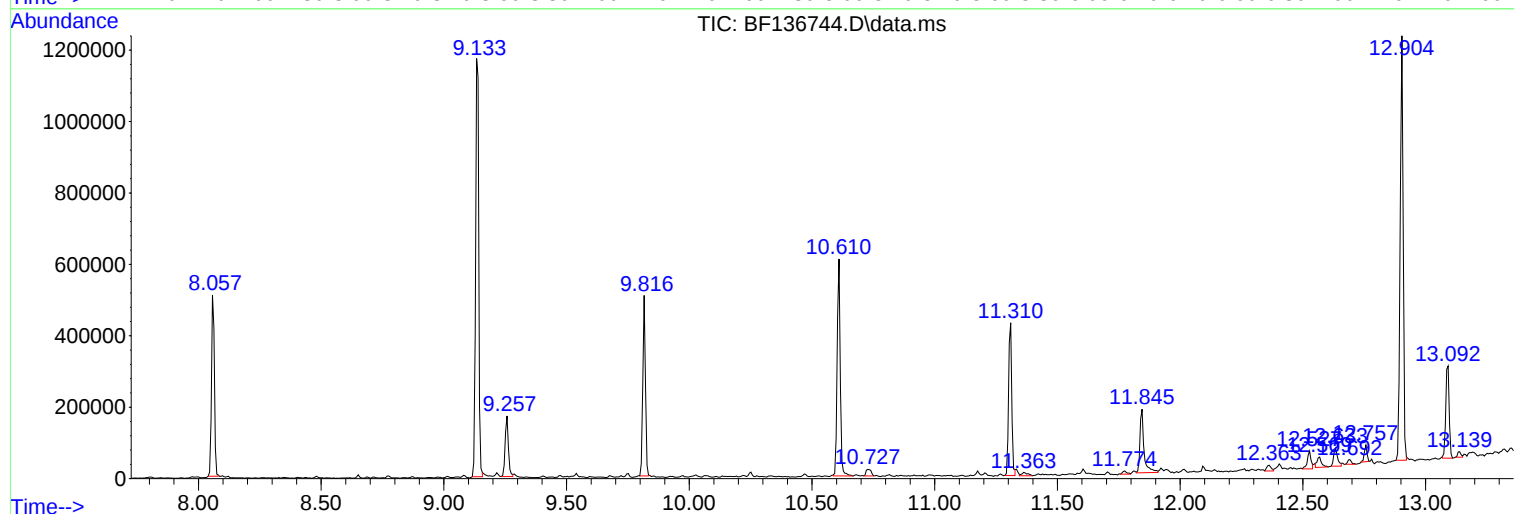
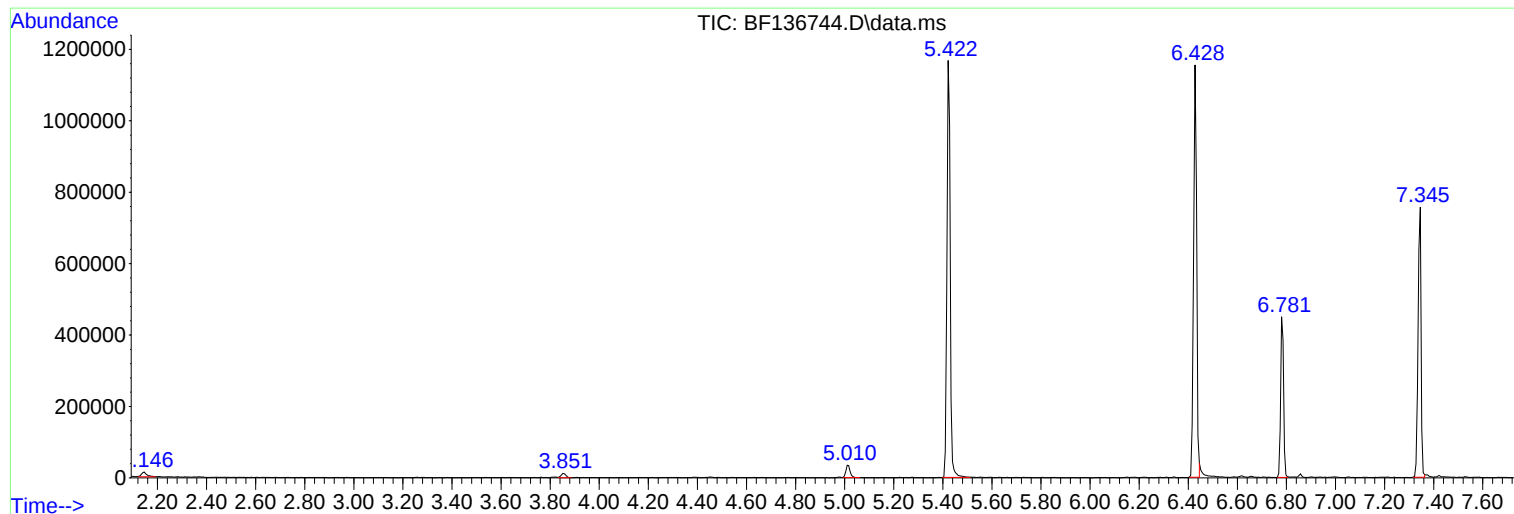
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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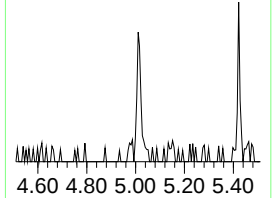
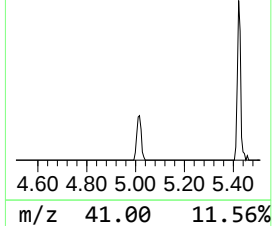
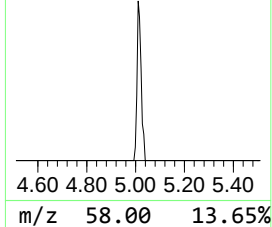
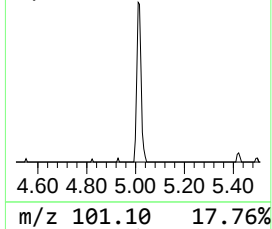
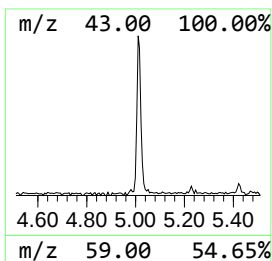
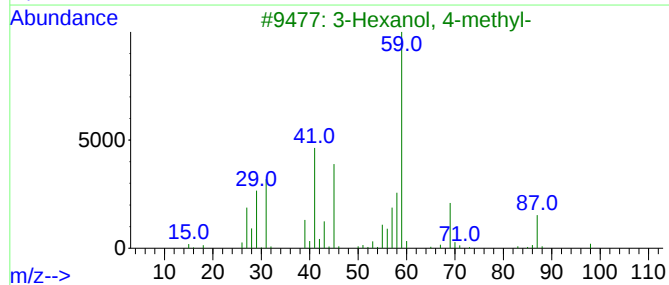
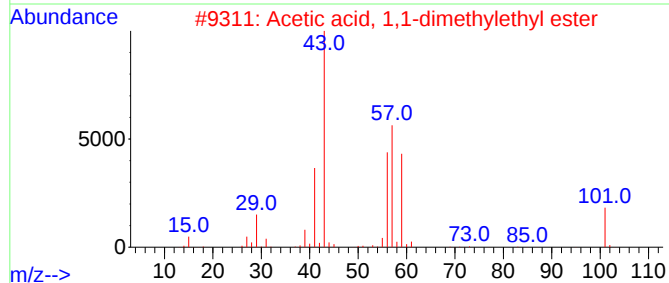
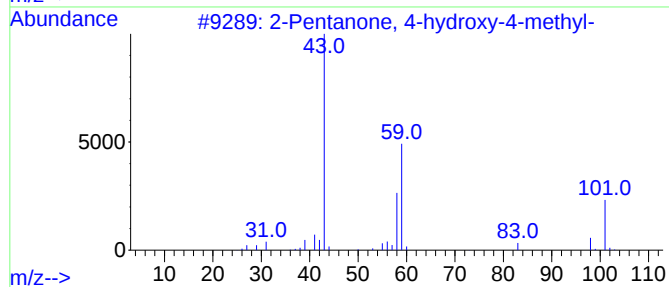
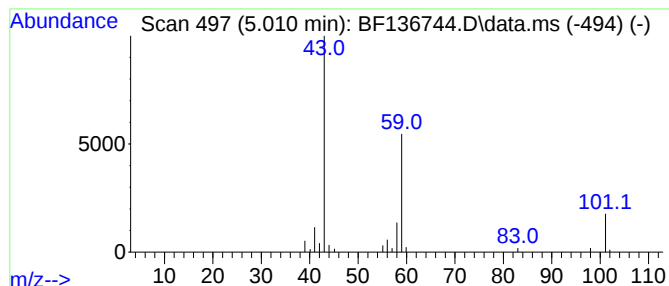
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	2.24 ng	41913	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		



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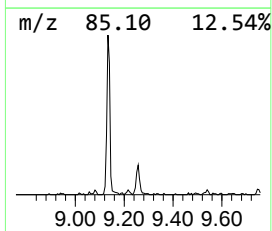
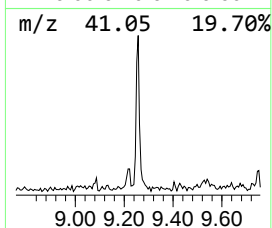
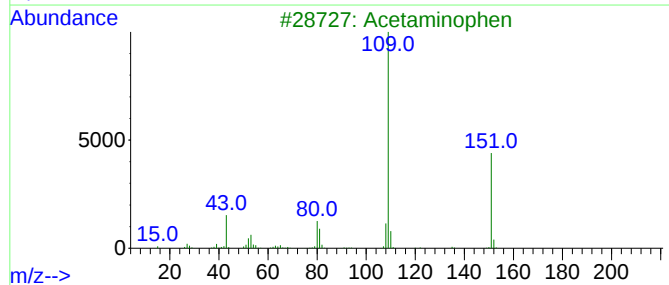
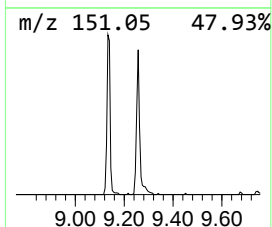
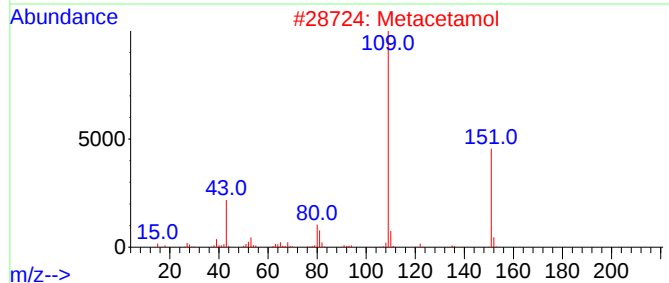
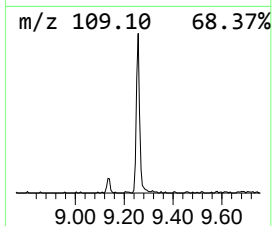
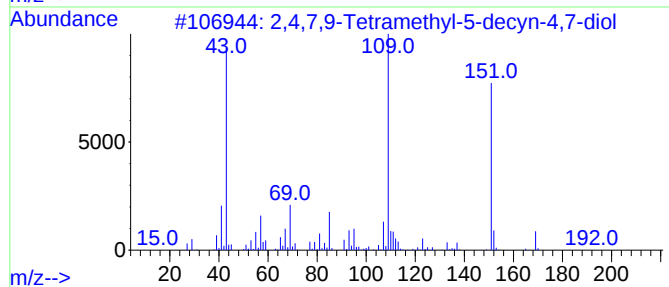
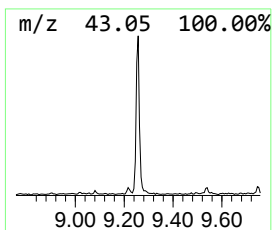
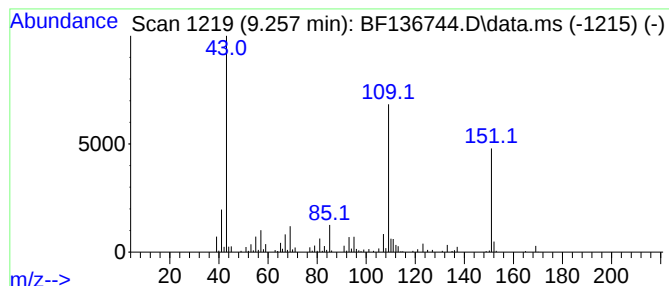
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	8.32 ng	155846	Acenaphthene-d10	9.816

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	Metacetamol	151	C8H9NO2	000621-42-1	58	
3	Acetaminophen	151	C8H9NO2	000103-90-2	53	
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	53	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	42	



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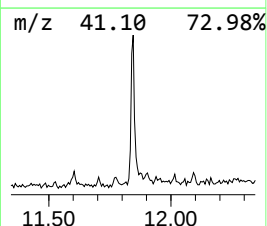
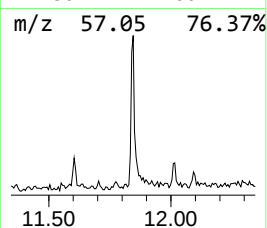
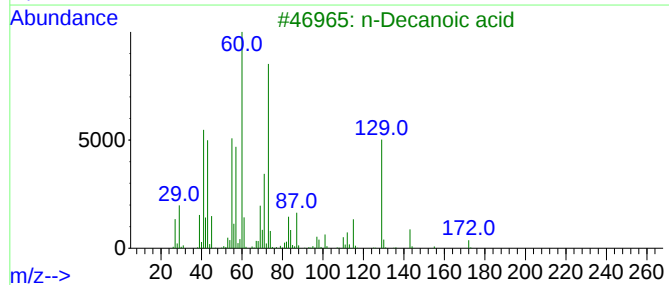
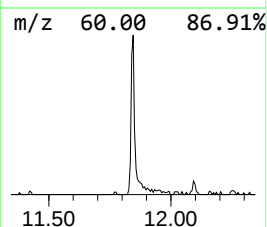
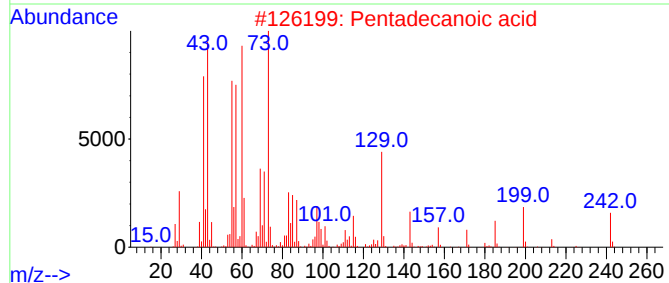
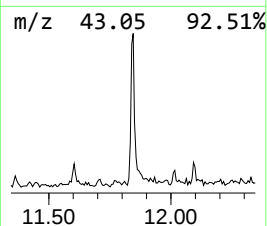
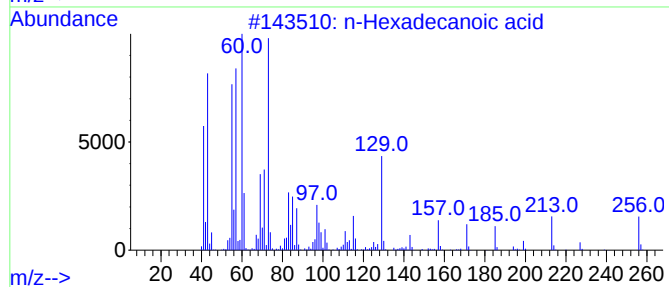
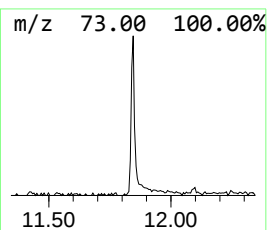
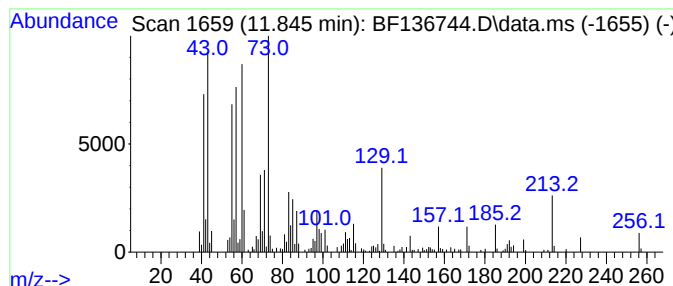
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	10.62 ng	203993	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Decanoic acid	172	C10H20O2	000334-48-5	92
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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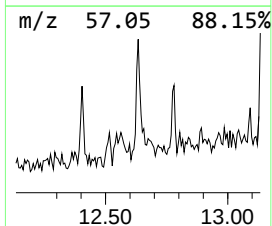
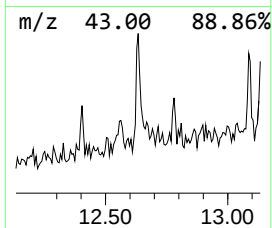
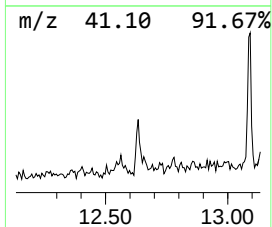
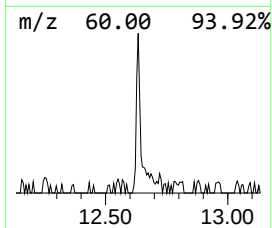
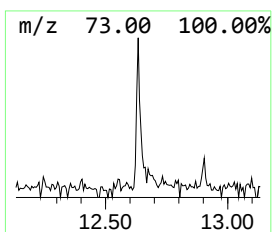
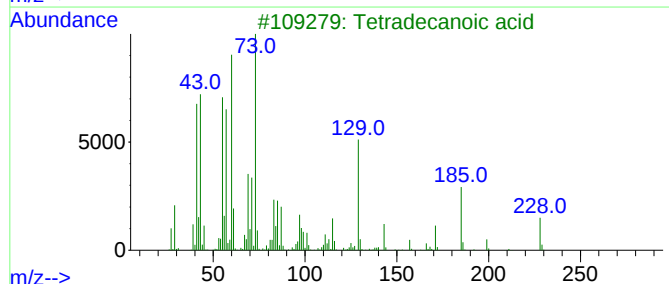
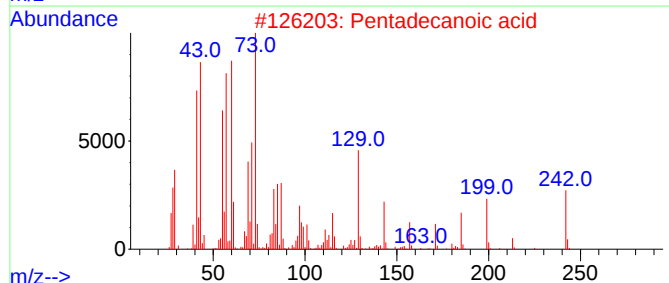
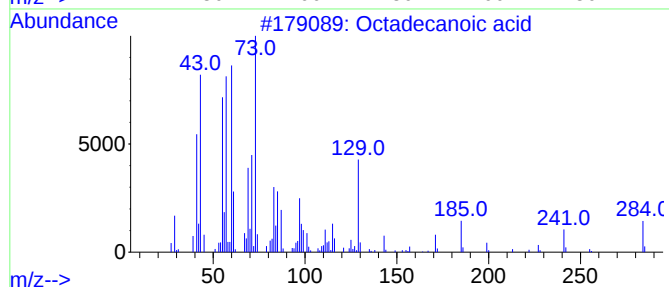
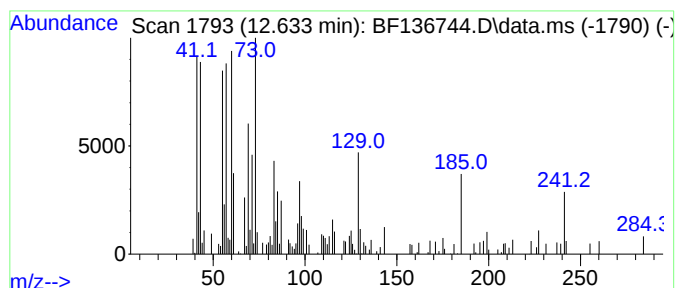
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	2.93 ng	56229	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	86
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	59
5			12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	53



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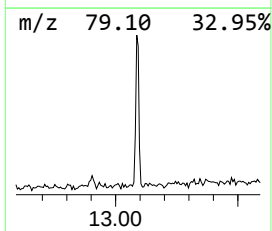
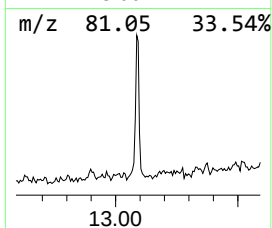
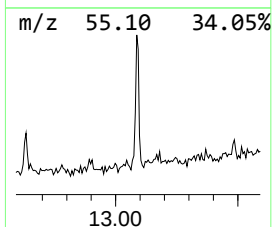
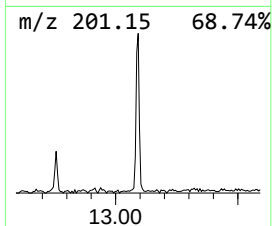
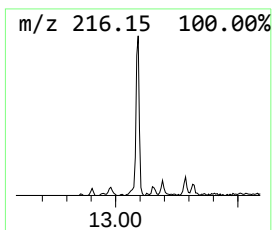
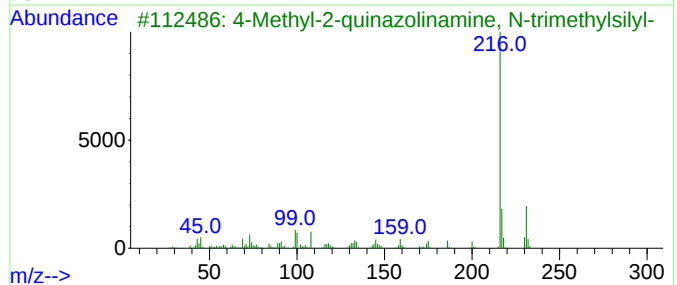
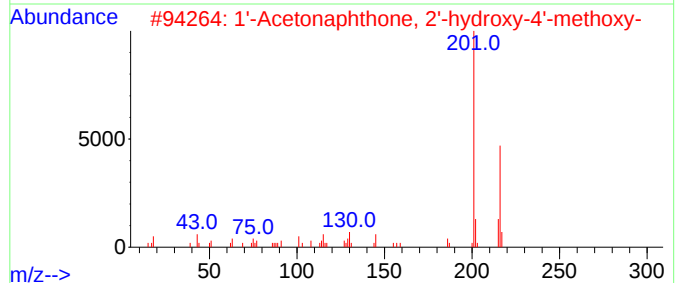
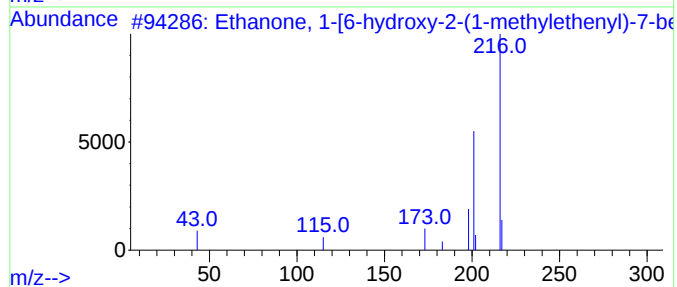
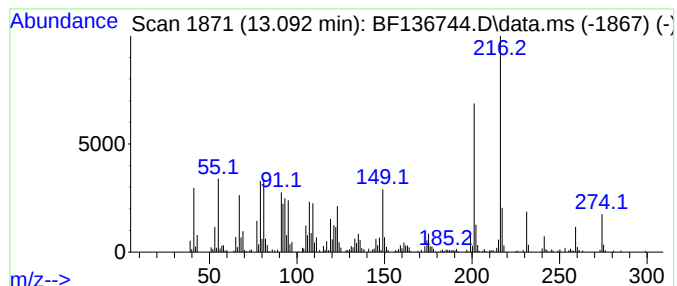
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Peak Number 6 unknown13.092 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.092	13.77 ng	251653	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-[6-hydroxy-2-(1-meth...	216	C13H12O3	055682-75-2	43
2			1'-Acetonaphthone, 2'-hydroxy-4'...	216	C13H12O3	005891-63-4	38
3			4-Methyl-2-quinazolinamine, N-tr...	231	C12H17N3Si	1010471-48-6	38
4			1,4-benzenediacetonitrile, 2,5-d...	216	C12H12N2O2	1000400-71-7	38
5			N-Ethyl-4,6-difluoro-2-pyrimidin...	231	C9H15F2N3Si	1000486-16-9	38



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Misc :
ALS Vial : 21 Sample Multiplier: 1

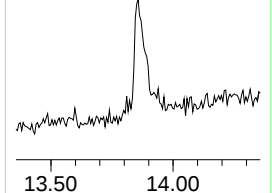
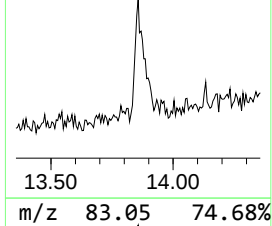
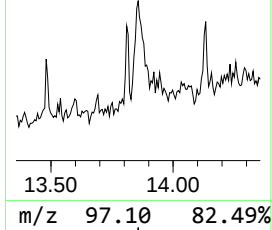
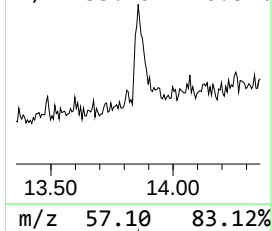
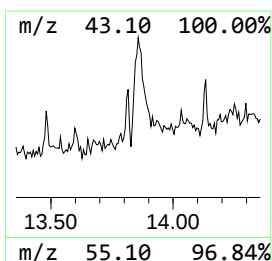
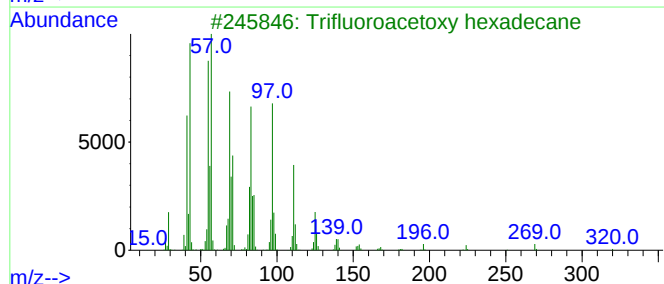
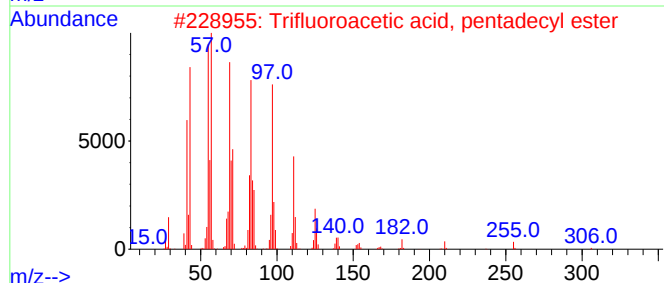
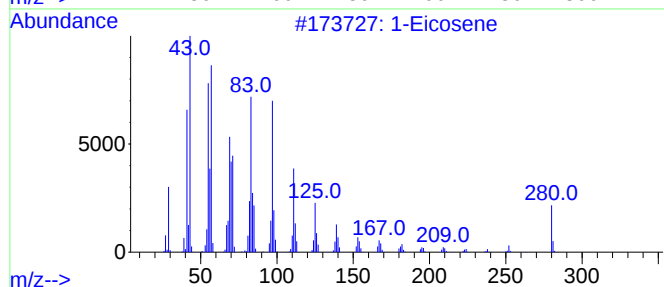
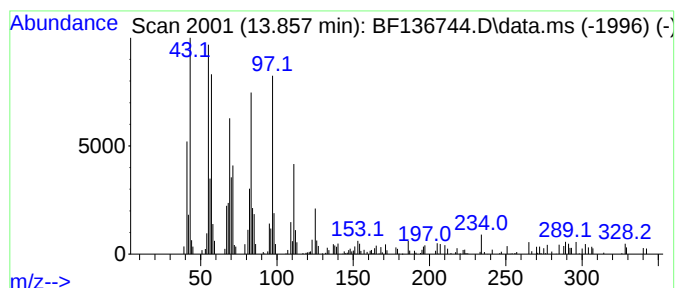
Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-6

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 7 1-Eicosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	10.98 ng	200696	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	93
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136744.D
Acq On : 27 Dec 2023 04:17
Operator : CG\JU
Sample : 05602-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-6

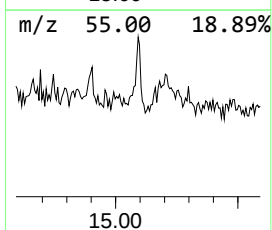
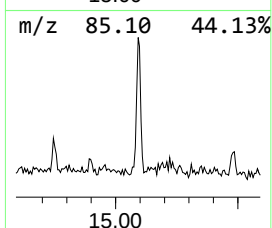
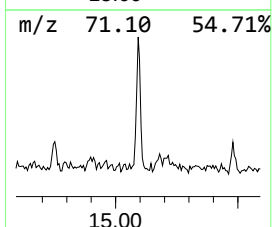
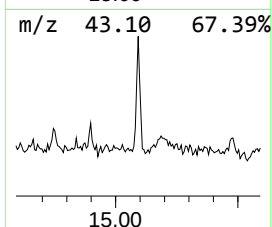
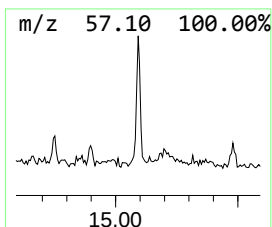
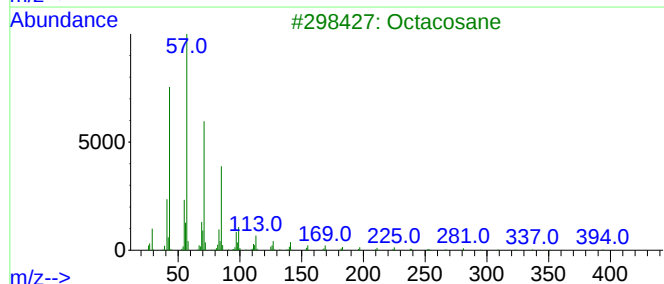
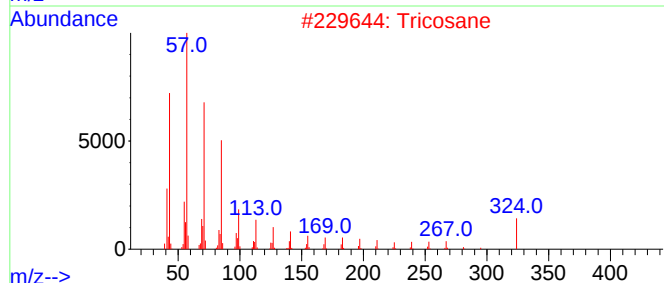
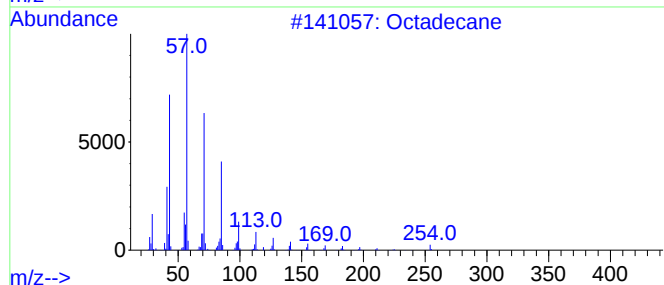
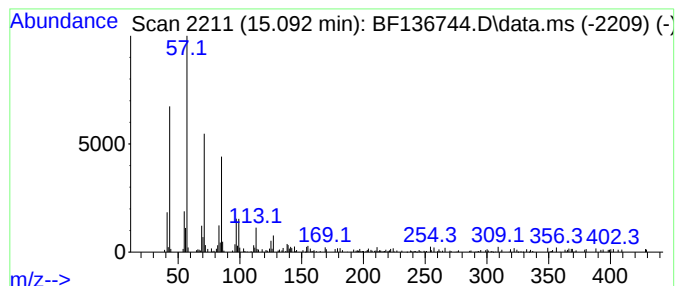
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	9.42 ng	103469	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	90
2			Tricosane	324	C23H48	000638-67-5	81
3			Octacosane	394	C28H58	000630-02-4	78
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74
5			3,5-Dimethyldodecane	198	C14H30	107770-99-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136744.D
Acq On : 27 Dec 2023 04:17
Operator : CG\JU
Sample : 05602-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-6

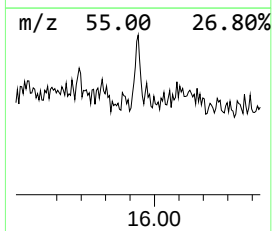
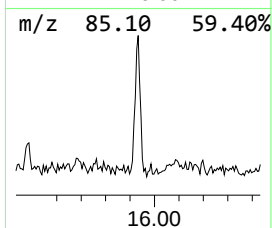
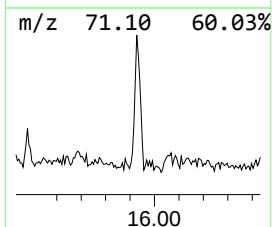
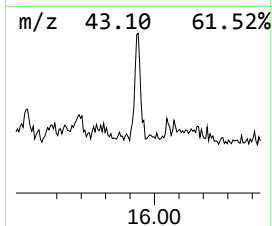
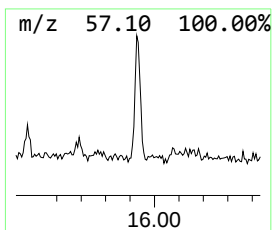
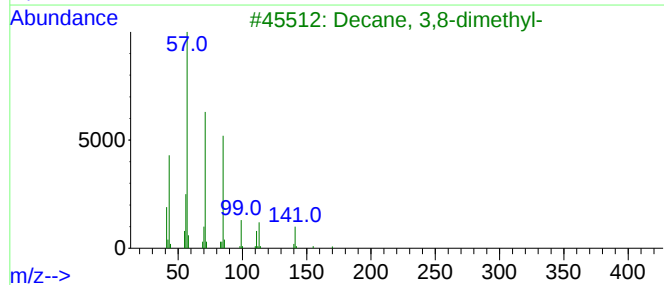
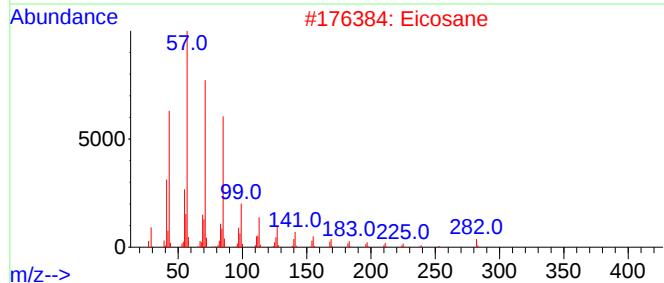
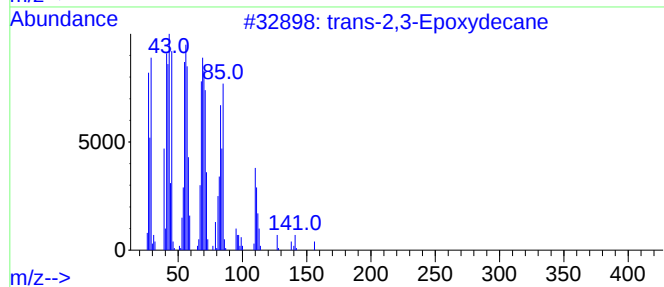
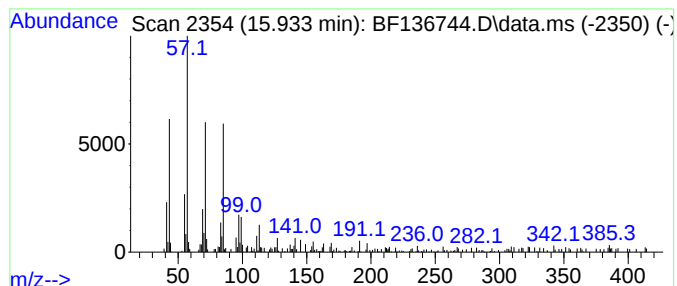
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 trans-2,3-Epoxydecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	8.10 ng	88954	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	92
2			Eicosane	282	C20H42	000112-95-8	78
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	74
5			Heneicosane	296	C21H44	000629-94-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136744.D
Acq On : 27 Dec 2023 04:17
Operator : CG\JU
Sample : 05602-11
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROUTE-4-TP-6

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
2-Pentanone, 4-...	5.010	2.2	ng	41913	1	6.781	374435	20.0
2,4,7,9-Tetrame...	9.257	8.3	ng	155846	3	9.816	374811	20.0
n-Hexadecanoic ...	11.845	10.6	ng	203993	4	11.310	384270	20.0
Octadecanoic acid	12.633	2.9	ng	56229	4	11.310	384270	20.0
unknown13.092	13.092	13.8	ng	251653	5	13.963	365529	20.0
1-Eicosene	13.857	11.0	ng	200696	5	13.963	365529	20.0
Octadecane	15.092	9.4	ng	103469	6	15.445	219578	20.0
trans-2,3-Epoxy...	15.933	8.1	ng	88954	6	15.445	219578	20.0