

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081324\
 Data File : BF138969.D
 Acq On : 13 Aug 2024 12:16
 Operator : RC/JU
 Sample : P3512-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 927-K1-SD-0.5-1.0-080724

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: BF138969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	21	rVB	541234	822312	71.06%	9.751%
2	3.422	222	226	247	rBV	4224	19525	1.69%	0.232%
3	5.069	501	506	521	rVB	44885	73569	6.36%	0.872%
4	5.475	570	575	599	rBV	791951	1075666	92.95%	12.755%
5	6.487	741	747	767	rBV	818756	1157272	100.00%	13.723%
6	6.839	802	807	813	rVB	205582	258913	22.37%	3.070%
7	7.404	897	903	921	rBV	545996	705033	60.92%	8.360%
8	7.657	942	946	955	rVB	16121	23060	1.99%	0.273%
9	8.116	1019	1024	1031	rBV	263302	334524	28.91%	3.967%
10	8.433	1074	1078	1090	rBV	32444	53187	4.60%	0.631%
11	9.192	1201	1207	1216	rBV	822263	1062958	91.85%	12.605%
12	9.580	1268	1273	1277	rBV2	11428	15291	1.32%	0.181%
13	9.869	1317	1322	1330	rVB	298516	370001	31.97%	4.387%
14	9.963	1333	1338	1343	rVB	26518	39822	3.44%	0.472%
15	10.510	1425	1431	1435	rBV	15174	20958	1.81%	0.249%
16	10.663	1452	1457	1467	rBV	506170	660917	57.11%	7.837%
17	10.775	1471	1476	1484	rVB2	46483	73502	6.35%	0.872%
18	11.239	1548	1555	1561	rVB	18209	28272	2.44%	0.335%
19	11.357	1570	1575	1588	rVB	274082	344923	29.80%	4.090%
20	11.804	1647	1651	1657	rVB	19227	23078	1.99%	0.274%
21	11.880	1659	1664	1674	rBV6	11355	23574	2.04%	0.280%
22	12.933	1838	1843	1849	rBV	586992	758915	65.58%	8.999%
23	13.839	1990	1997	2010	rBV7	11604	43367	3.75%	0.514%
24	13.998	2019	2024	2036	rVB	150962	198131	17.12%	2.349%
25	15.074	2198	2207	2214	rVB2	27918	44831	3.87%	0.532%
26	15.462	2267	2273	2281	rBV	111270	176426	15.24%	2.092%
27	15.874	2337	2343	2349	rBV2	13106	25052	2.16%	0.297%

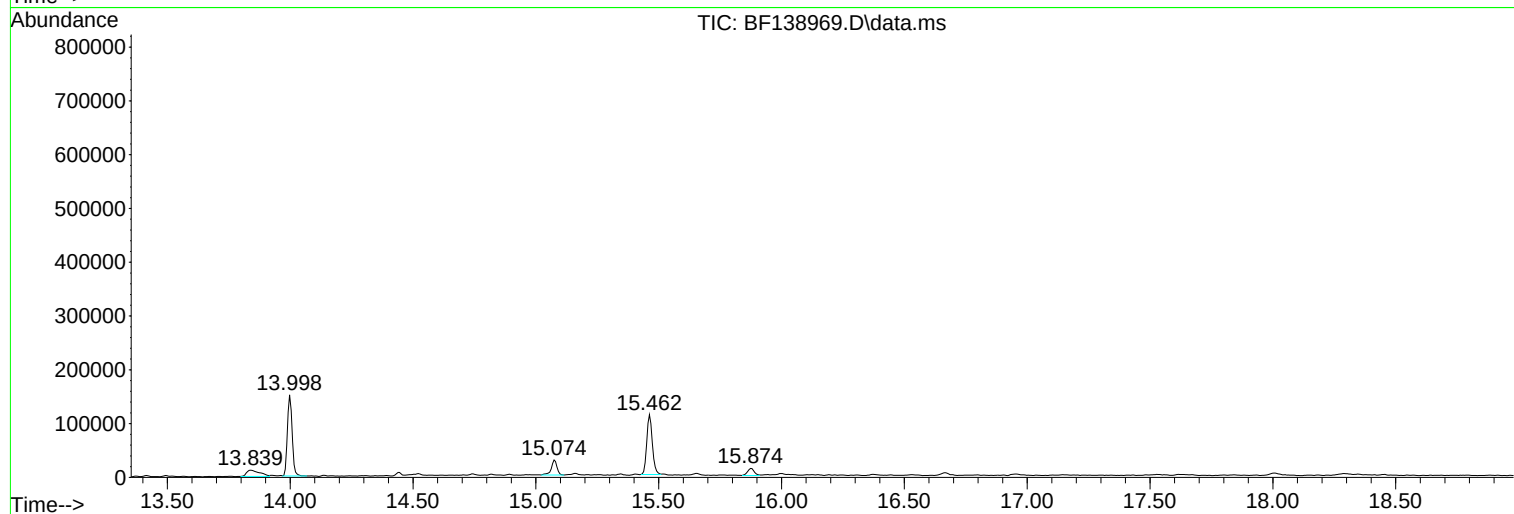
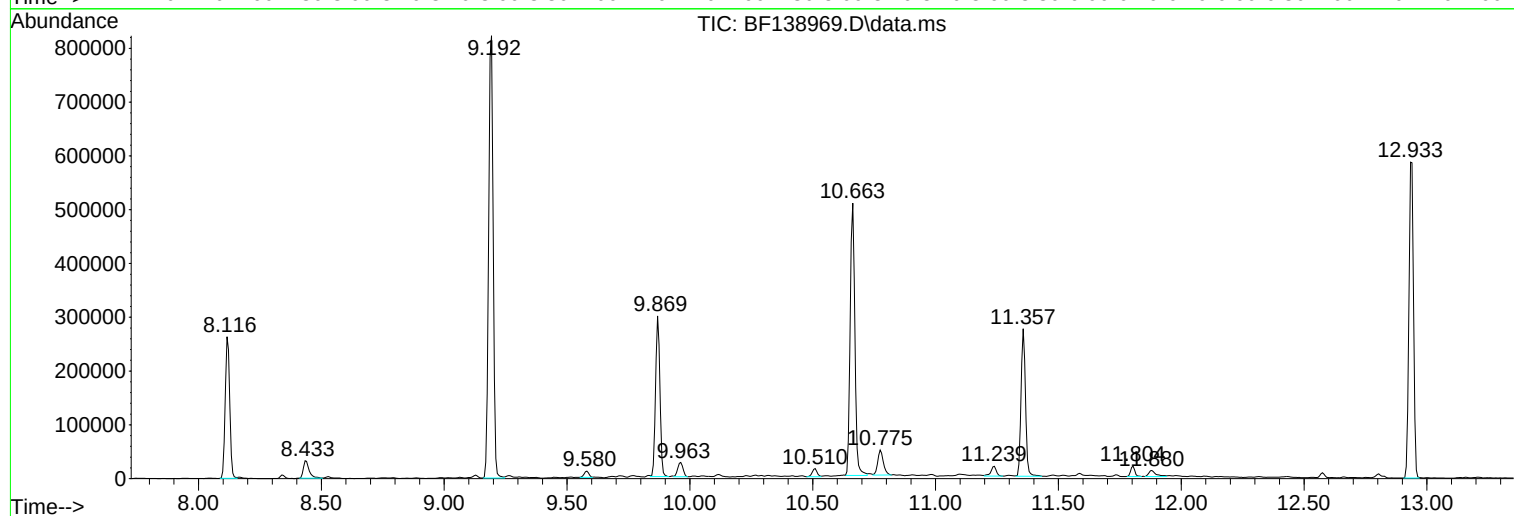
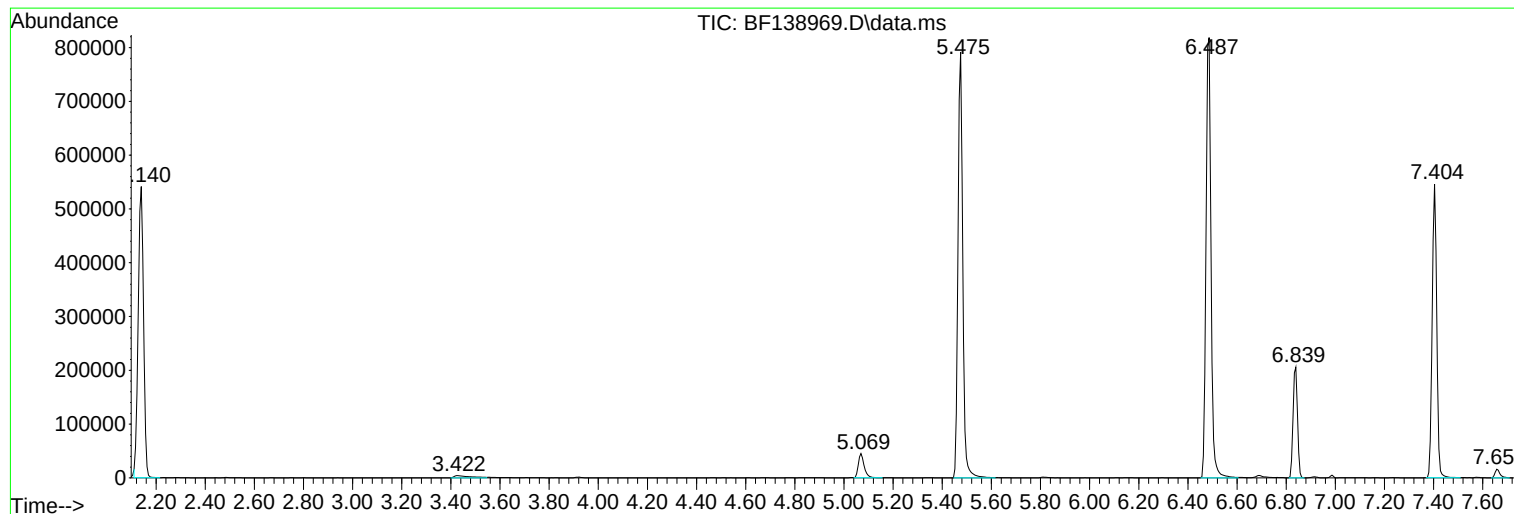
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Instrument :
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ClientSampleId :
927-K1-SD-0.5-1.0-080724

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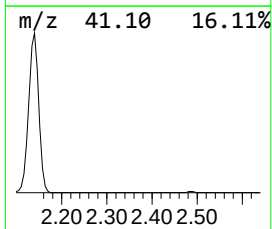
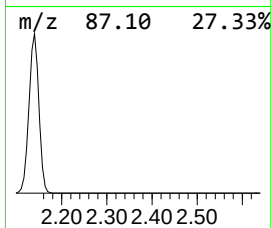
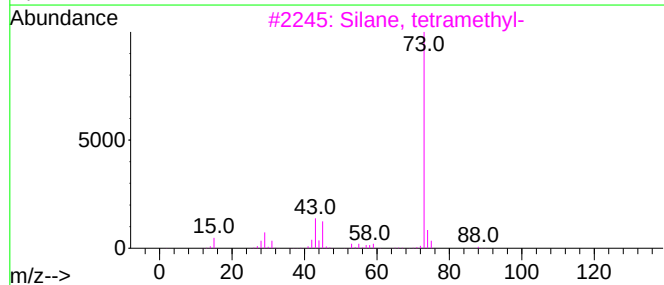
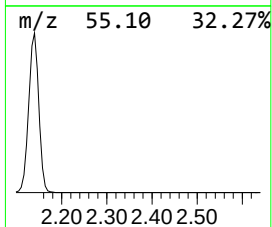
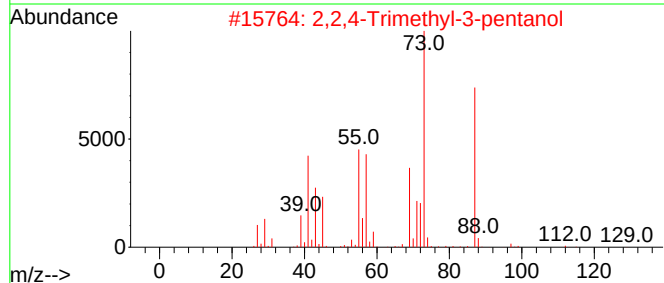
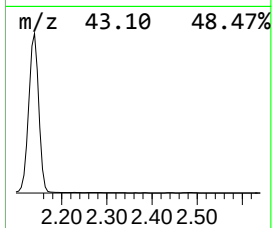
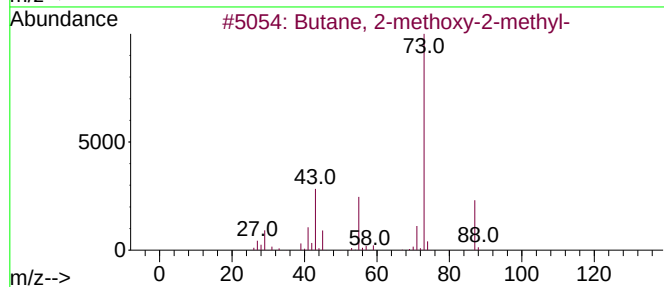
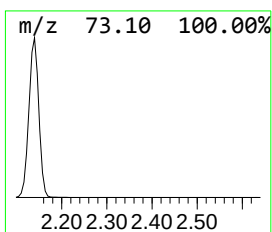
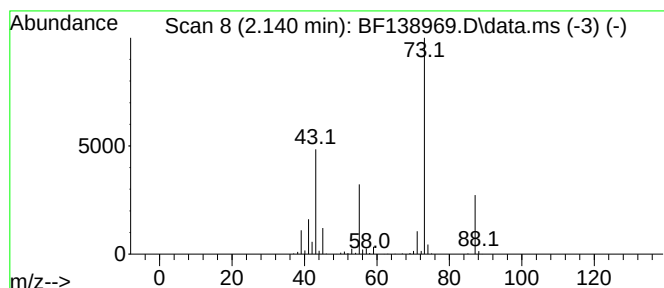
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	63.52 ng	822312	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9



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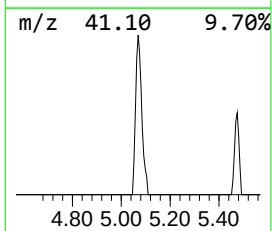
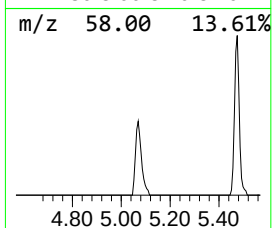
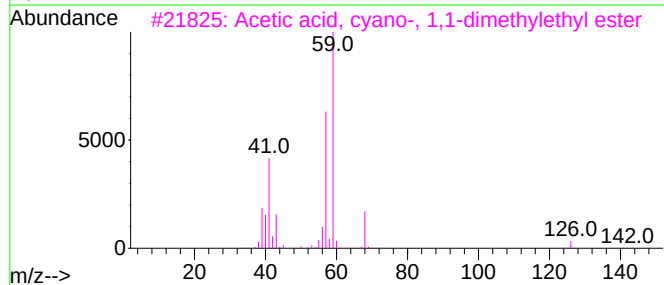
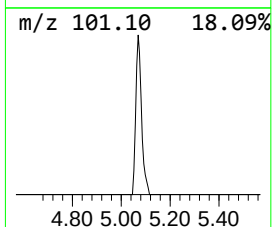
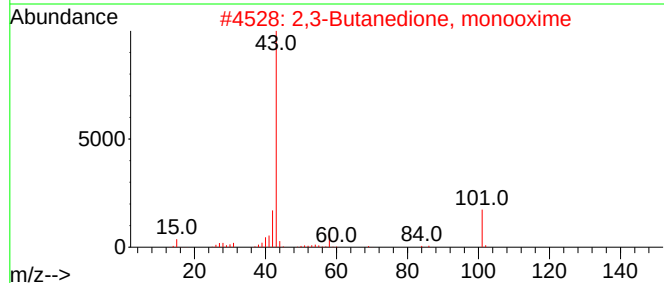
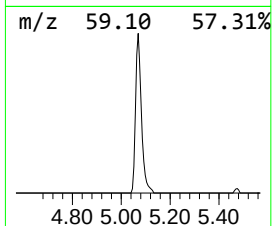
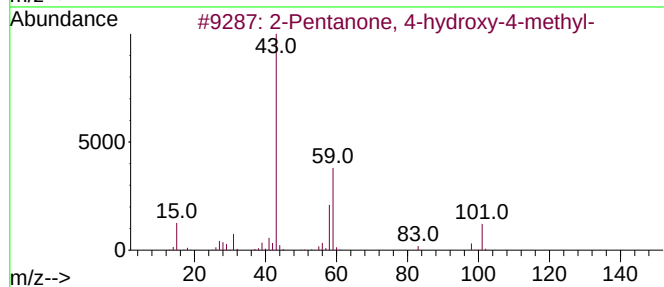
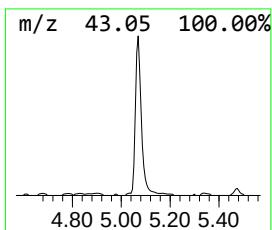
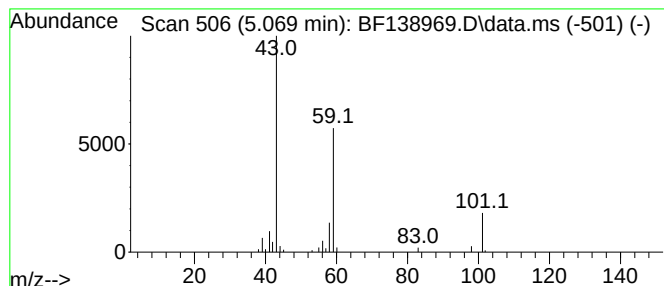
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	5.68 ng	73569	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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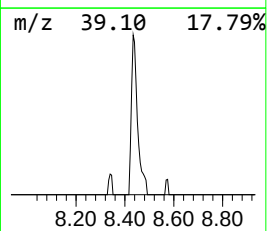
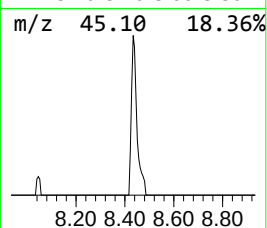
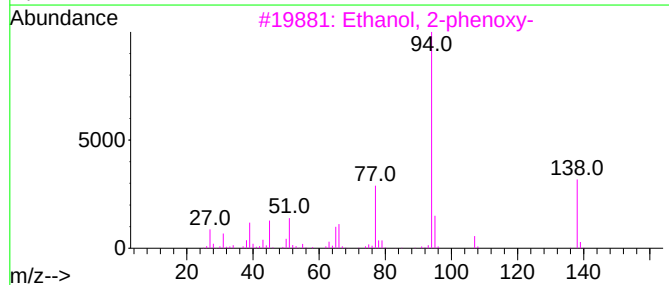
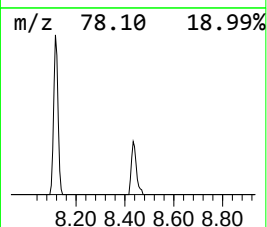
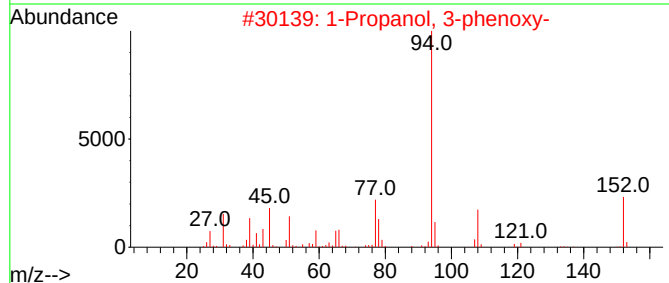
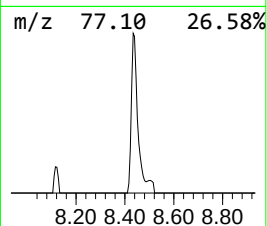
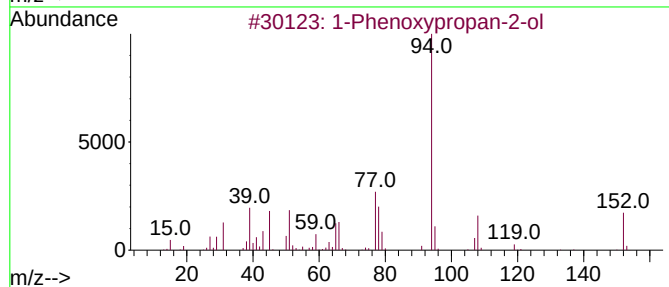
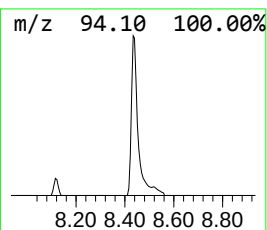
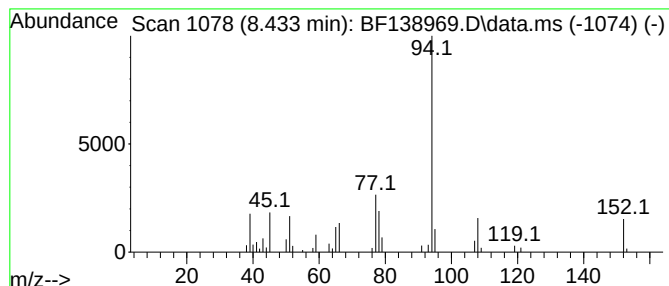
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.18 ng	53187	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5			Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53



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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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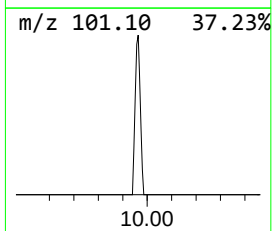
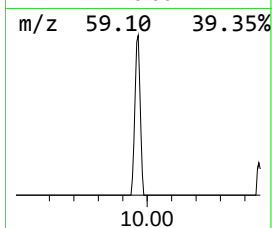
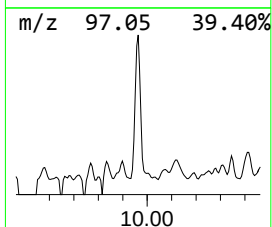
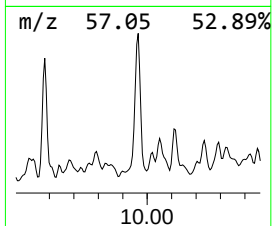
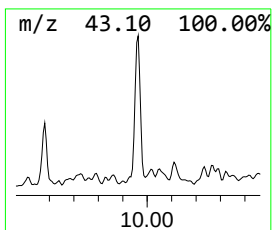
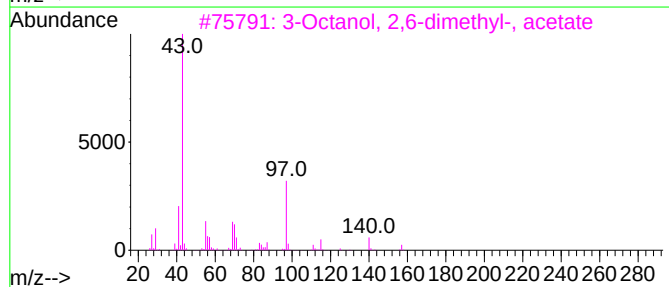
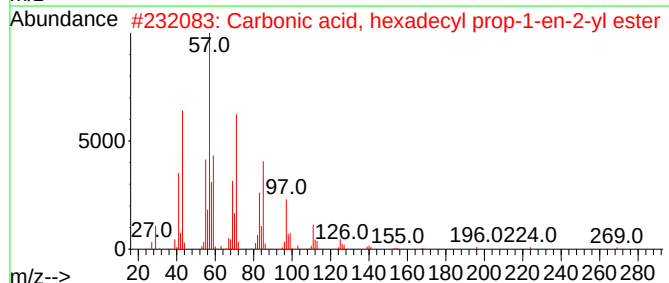
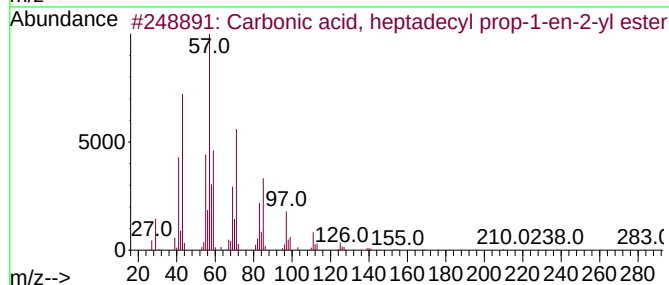
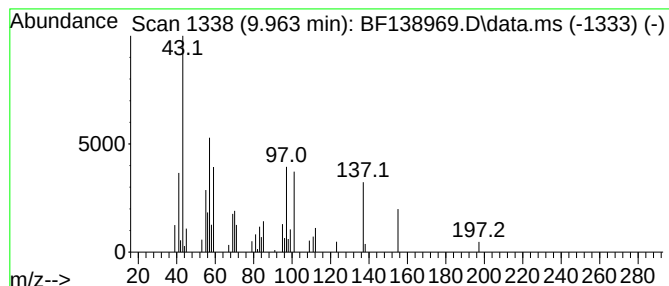
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown9.963 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	2.15 ng	39822	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, heptadecyl prop-1...	340	C21H40O3	1000382-90-2	37
2			Carbonic acid, hexadecyl prop-1...	326	C20H38O3	1000382-90-3	37
3			3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	14
4			(1S,2R,4R,7R)-4-Isopropyl-7-meth...	168	C10H16O2	001619-26-7	14
5			2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10



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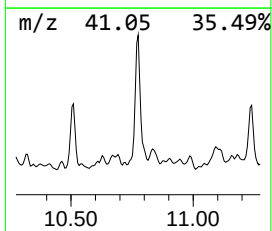
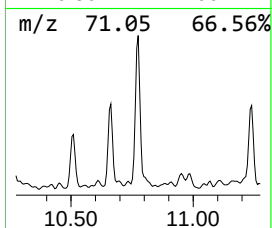
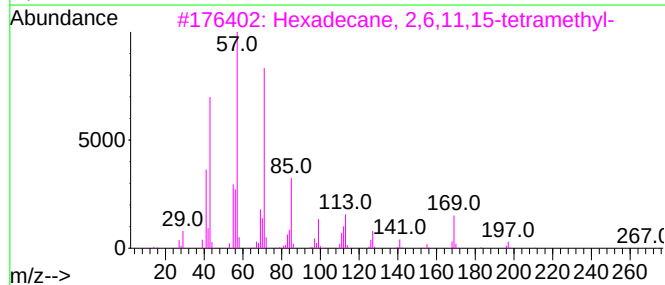
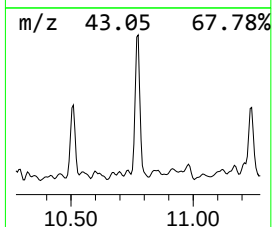
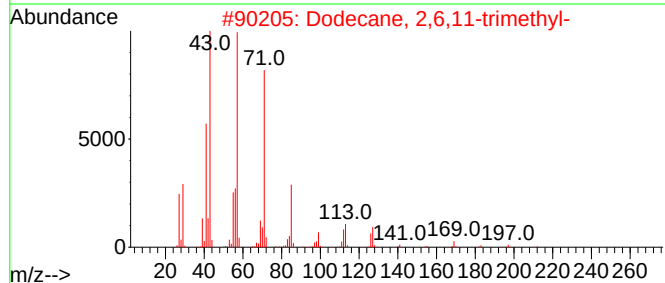
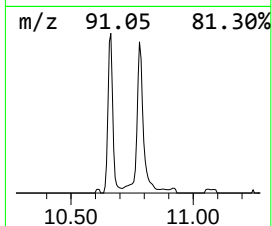
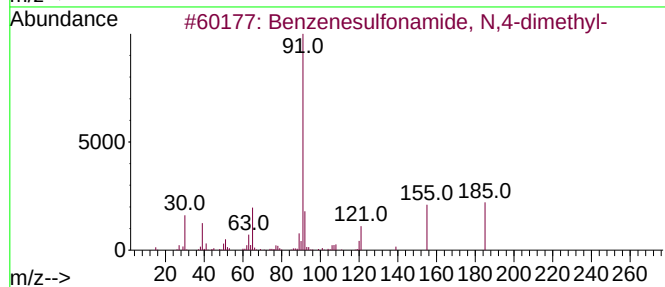
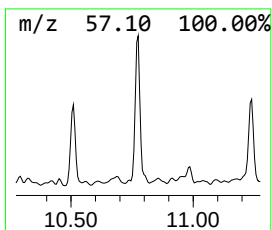
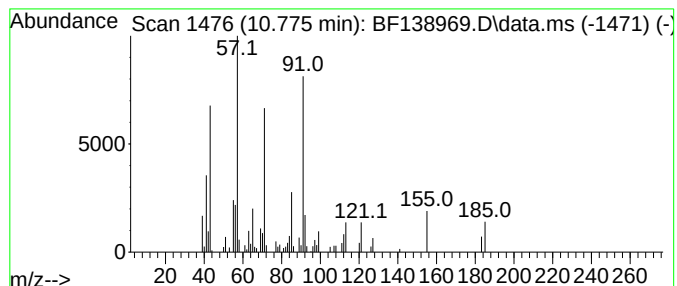
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown10.775 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	4.26 ng	73502	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	46
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	41
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	41
4			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	38
5			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	38



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927-K1-SD-0.5-1.0-080724

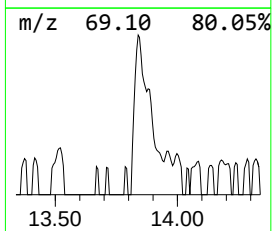
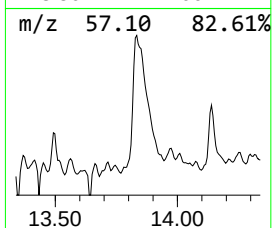
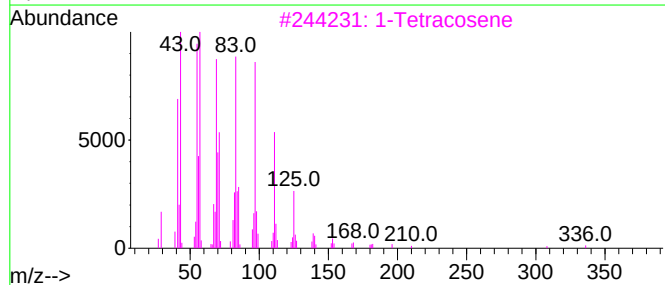
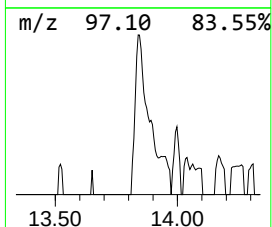
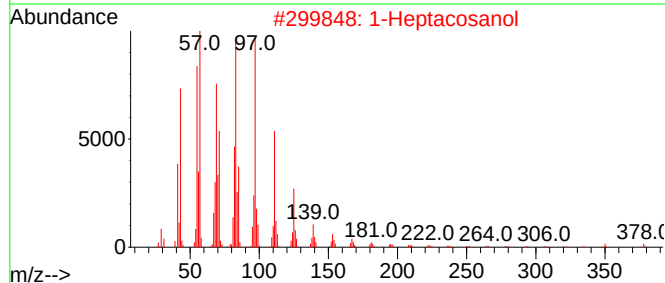
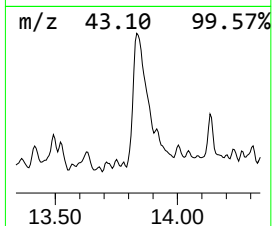
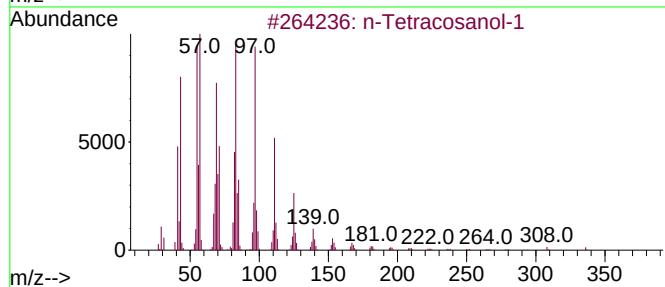
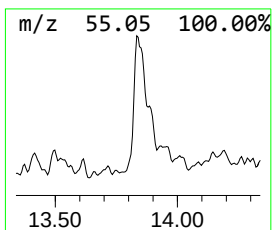
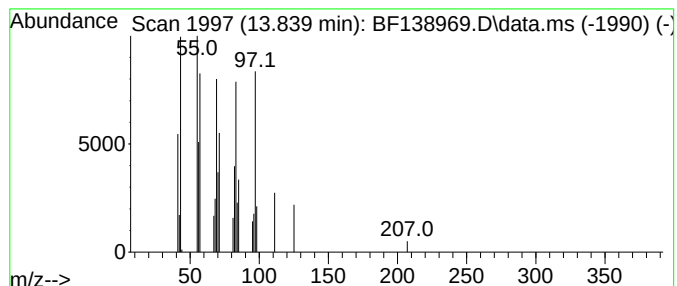
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	4.38 ng	43367	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			1-Heptacosanol	396	C27H56O	002004-39-9	91
3			1-Tetracosene	336	C24H48	010192-32-2	87
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5			Behenic alcohol	326	C22H46O	000661-19-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081324\
Data File : BF138969.D
Acq On : 13 Aug 2024 12:16
Operator : RC/JU
Sample : P3512-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

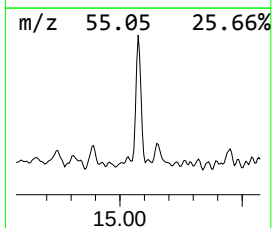
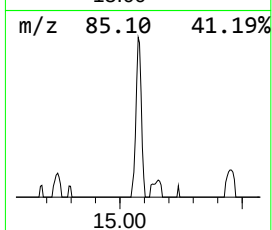
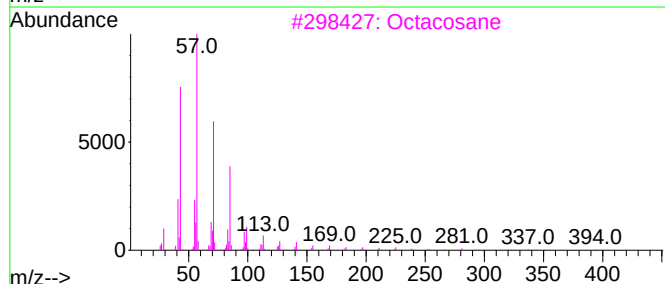
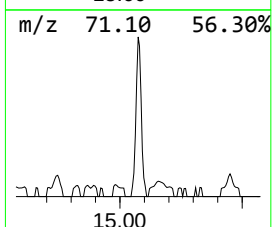
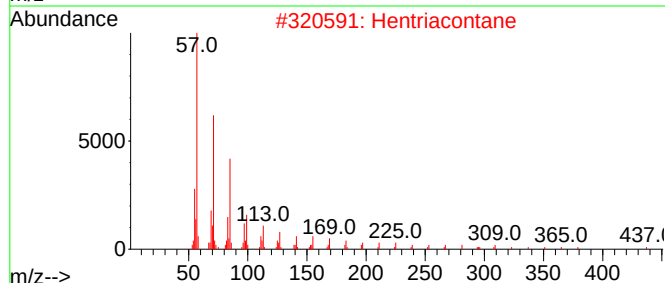
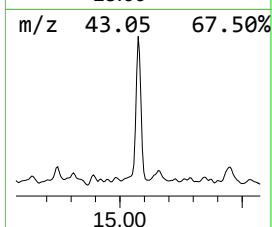
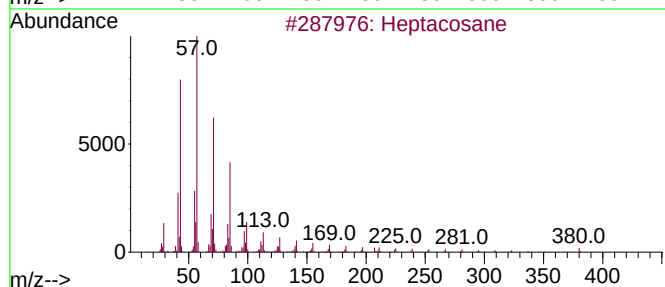
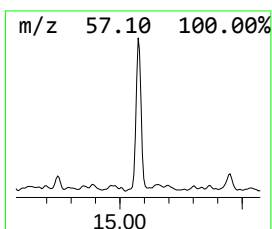
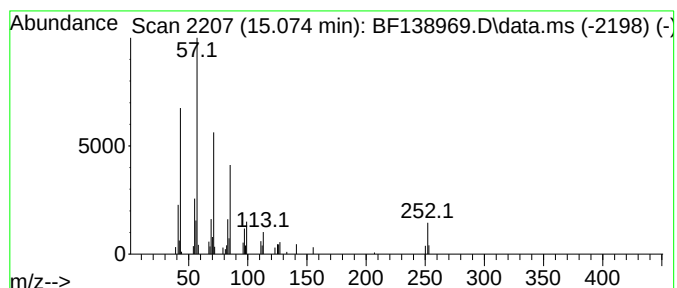
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927-K1-SD-0.5-1.0-080724

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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 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.074	5.08 ng	44831	Perylene-d12	15.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Hentriacontane	437	C31H64	000630-04-6	87
3	Octacosane	394	C28H58	000630-02-4	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5	Tetratetracontane	619	C44H90	007098-22-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081324\
Data File : BF138969.D
Acq On : 13 Aug 2024 12:16
Operator : RC/JU
Sample : P3512-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
927-K1-SD-0.5-1.0-080724

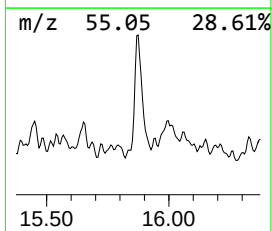
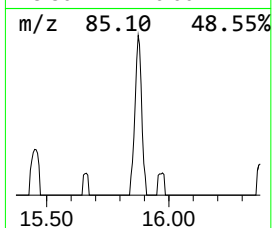
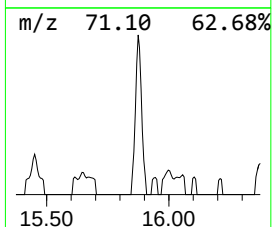
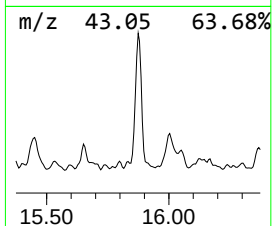
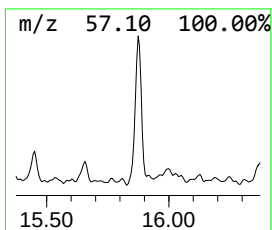
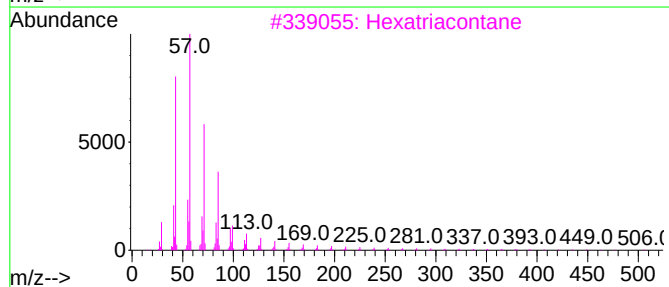
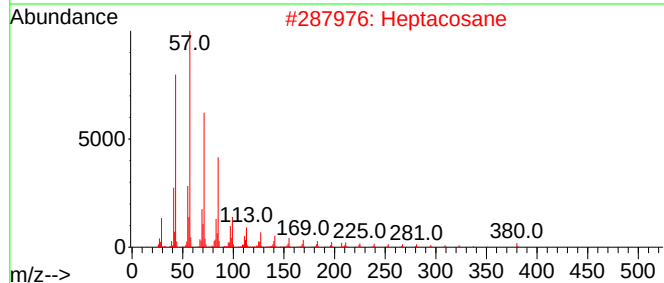
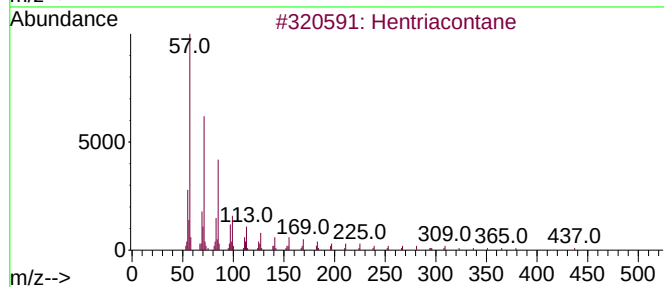
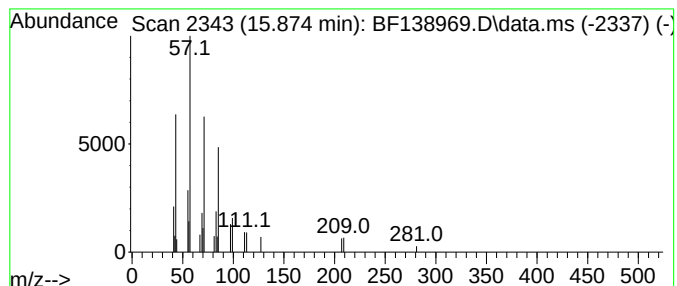
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	2.84 ng	25052	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	87
2			Heptacosane	380	C27H56	000593-49-7	87
3			Hexatriacontane	507	C36H74	000630-06-8	86
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
5			Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081324\
Data File : BF138969.D
Acq On : 13 Aug 2024 12:16
Operator : RC/JU
Sample : P3512-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
927-K1-SD-0.5-1.0-080724

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
Butane, 2-metho...	2.140	63.5	ng	822312	1	6.839	258913	20.0
2-Pentanone, 4-...	5.069	5.7	ng	73569	1	6.839	258913	20.0
1-Phenoxypropan...	8.433	3.2	ng	53187	2	8.116	334524	20.0
unknown9.963	9.963	2.1	ng	39822	3	9.869	370001	20.0
unknown10.775	10.775	4.3	ng	73502	4	11.357	344923	20.0
n-Tetracosanol-1	13.839	4.4	ng	43367	5	13.998	198131	20.0
Heptacosane	15.074	5.1	ng	44831	6	15.462	176426	20.0
Hentriacontane	15.874	2.8	ng	25052	6	15.462	176426	20.0