

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
 Data File : BM039150.D
 Acq On : 24 Mar 2023 20:22
 Operator : CG/JU
 Sample : 02069-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 API-3-4

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_M\Methods\8270-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039150.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	291	298	305	rBV	720655	1033239	8.22%	1.627%
2	5.505	371	377	386	rVB	2555740	3602410	28.66%	5.673%
3	7.110	643	650	662	rVB	1436017	2247793	17.88%	3.540%
4	7.946	784	792	800	rBV	818344	1300742	10.35%	2.049%
5	9.116	984	991	1007	rBV	3032888	4992852	39.72%	7.863%
6	10.763	1263	1271	1283	rVB	1029803	1743908	13.87%	2.746%
7	12.275	1523	1528	1541	rVB	72822	149660	1.19%	0.236%
8	13.216	1679	1688	1695	rBV	7107608	10344343	82.29%	16.291%
9	14.404	1886	1890	1895	rBV3	123658	190245	1.51%	0.300%
10	14.592	1916	1922	1927	rBV	1541210	2215731	17.63%	3.490%
11	14.810	1956	1959	1965	rBV4	65025	134780	1.07%	0.212%
12	15.198	2021	2025	2029	rBV4	98813	167467	1.33%	0.264%
13	15.428	2059	2064	2069	rBV5	75009	156051	1.24%	0.246%
14	15.545	2081	2084	2093	rVB5	202748	386218	3.07%	0.608%
15	15.686	2104	2108	2117	rBV5	123444	208572	1.66%	0.328%
16	15.951	2148	2153	2158	rBV	1224679	1673897	13.32%	2.636%
17	16.080	2169	2175	2188	rVB	5461771	7954450	63.28%	12.527%
18	16.510	2244	2248	2256	rVB2	220073	341631	2.72%	0.538%
19	16.839	2300	2304	2317	rVB	1065194	1434943	11.42%	2.260%
20	17.333	2384	2388	2394	rBV	1646580	2352203	18.71%	3.704%
21	18.233	2537	2541	2553	rBV	972906	1417542	11.28%	2.232%
22	19.510	2754	2758	2766	rBV	526626	736193	5.86%	1.159%
23	19.957	2829	2834	2840	rBV	9871185	12570422	100.00%	19.797%
24	20.868	2987	2989	2993	rVB	214721	232759	1.85%	0.367%
25	21.221	3046	3049	3054	rVB	444096	492871	3.92%	0.776%
26	21.515	3095	3099	3106	rVB2	2016834	2595012	20.64%	4.087%
27	23.945	3506	3512	3520	rVB2	1396686	2820295	22.44%	4.442%

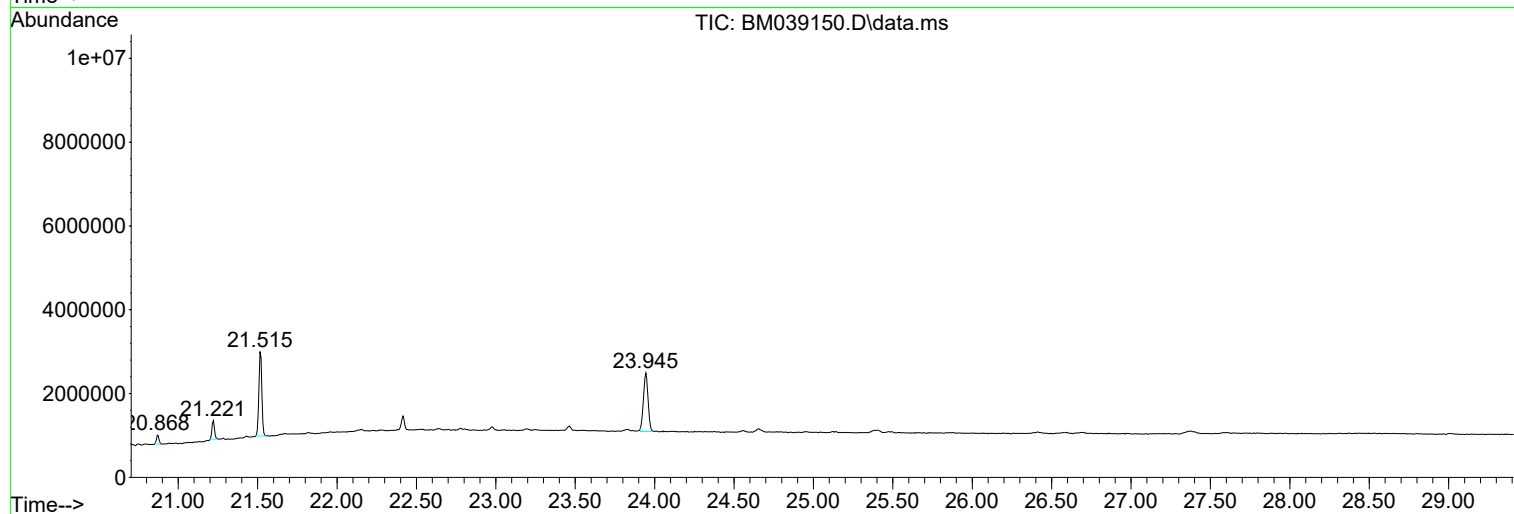
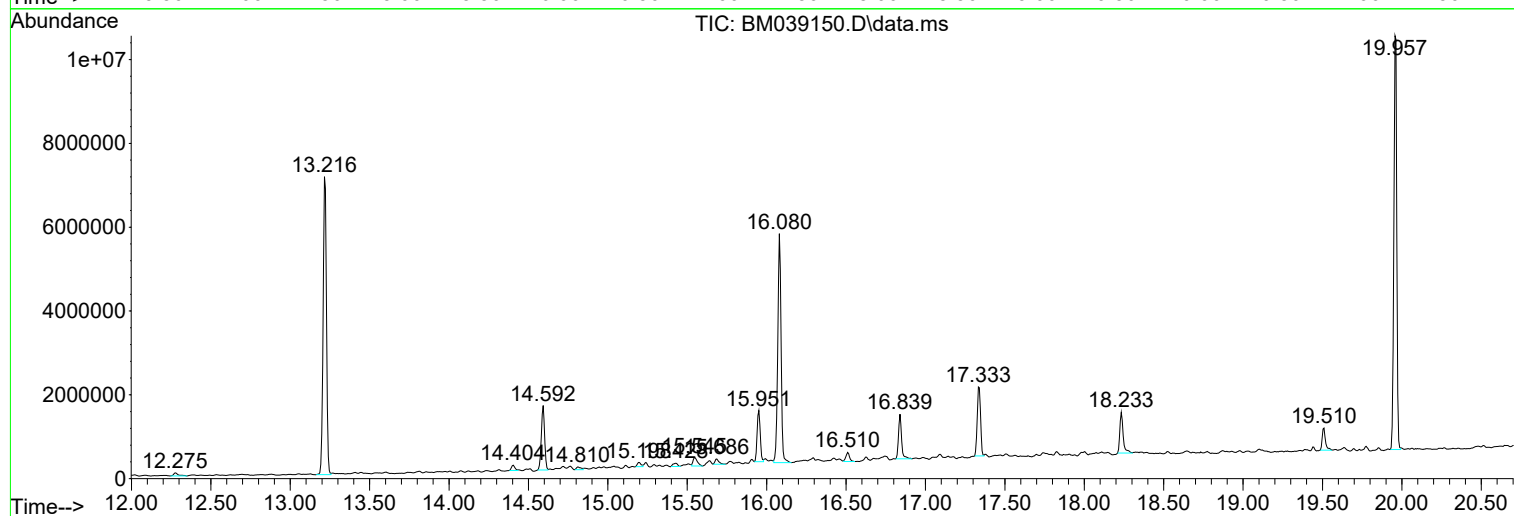
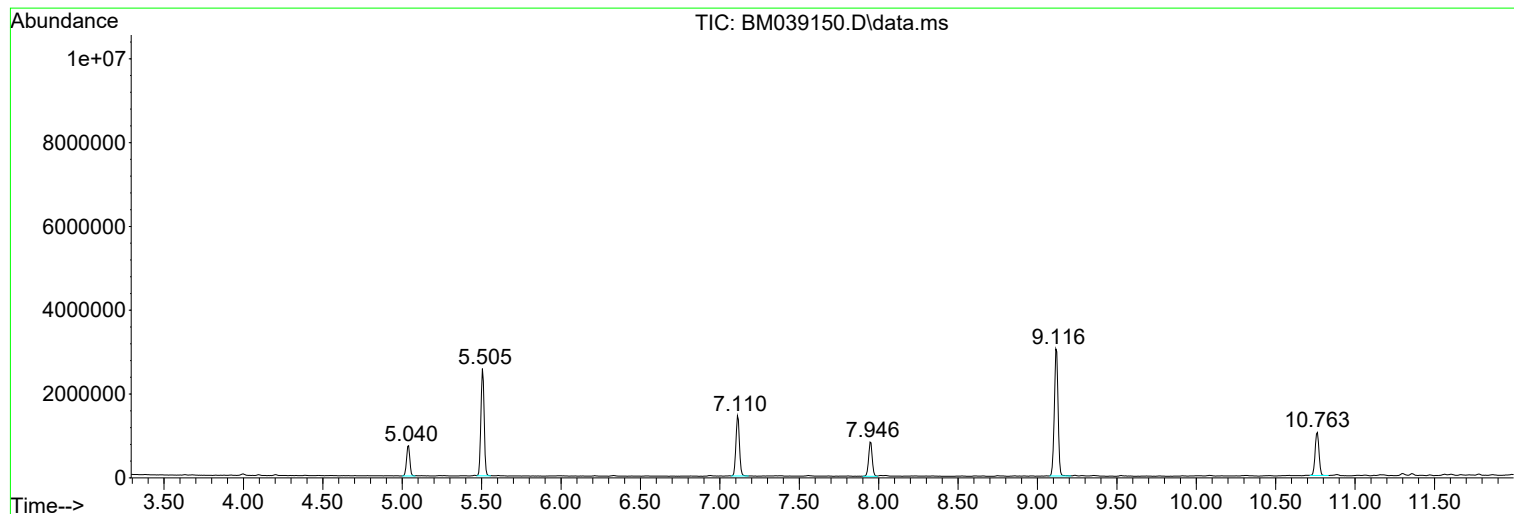
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BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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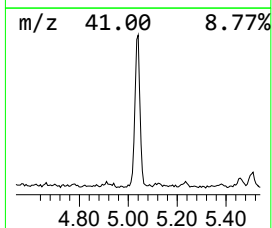
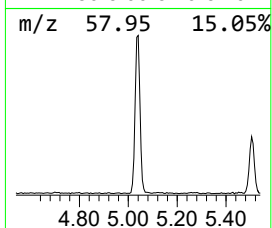
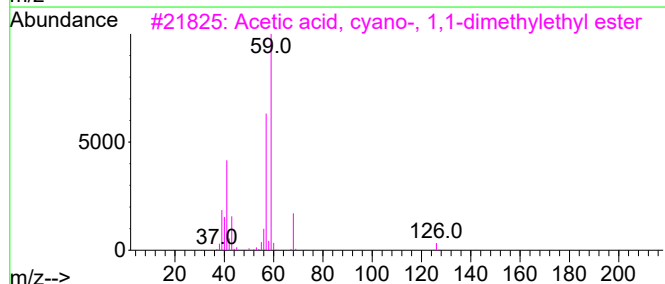
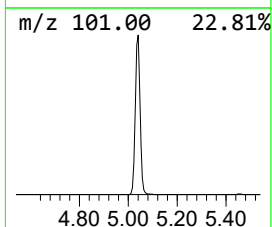
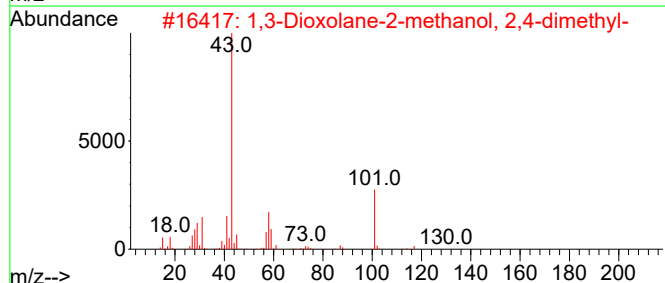
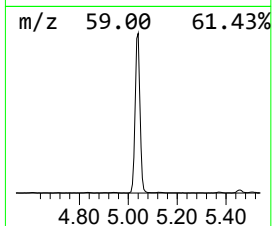
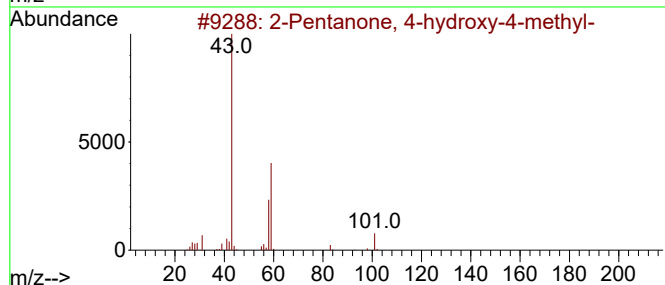
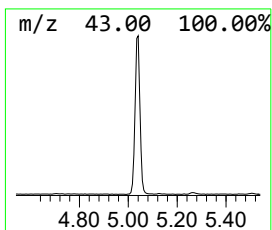
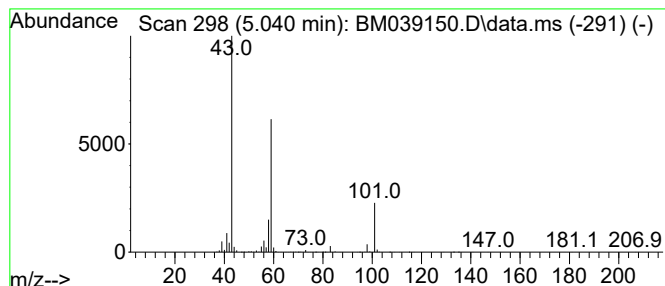
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.040	15.89 ng	1033240	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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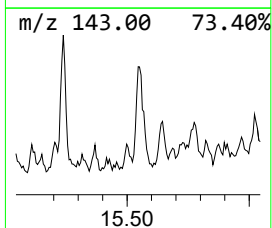
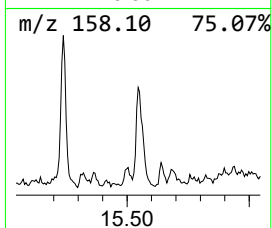
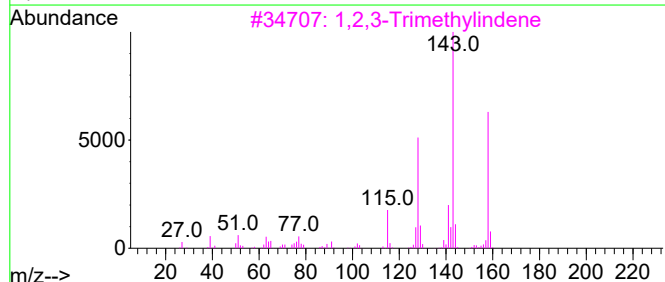
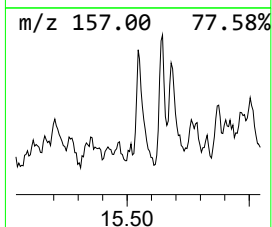
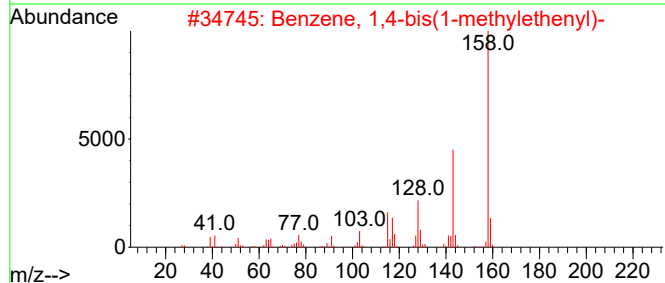
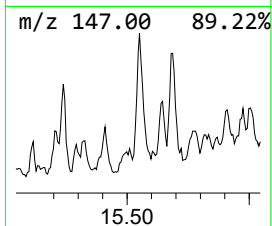
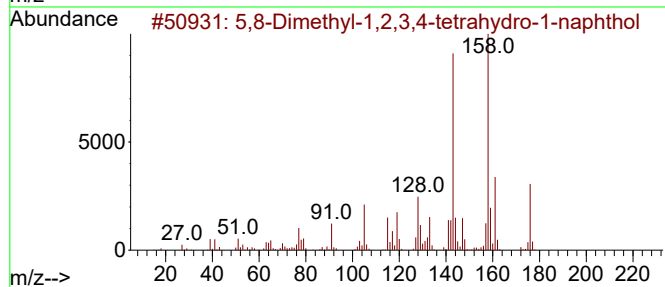
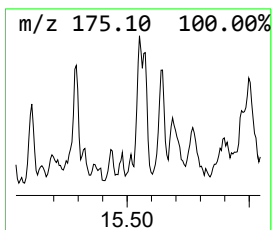
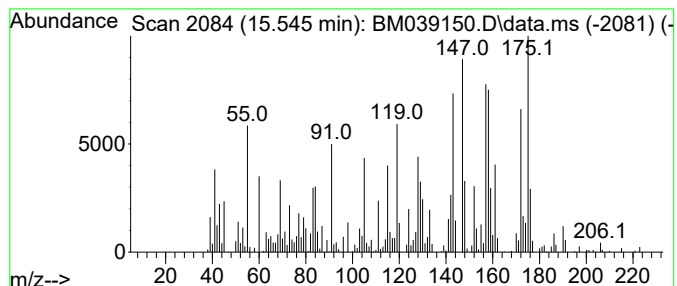
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Peak Number 2 unknown15.545 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	3.49 ng	386218	Acenaphthene-d10	14.592

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5,8-Dimethyl-1,2,3,4-tetrahydro-...	176	C12H16O	032820-12-5	30
2		Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	30
3		1,2,3-Trimethylindene	158	C12H14	004773-83-5	30
4		1H-Indene, 1,1,3-trimethyl-	158	C12H14	002177-45-9	25
5		1,3,5-Cycloheptatriene, 2,4-diet...	176	C13H20	1000156-99-6	18



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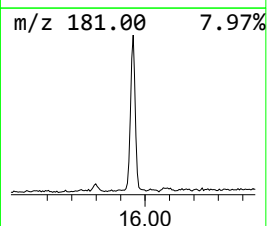
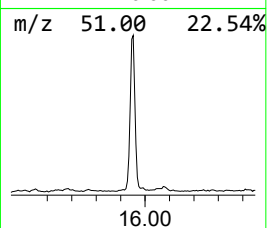
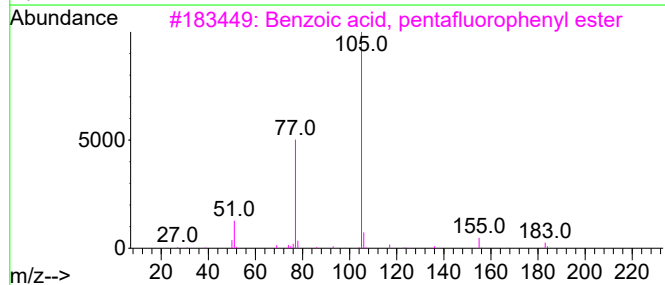
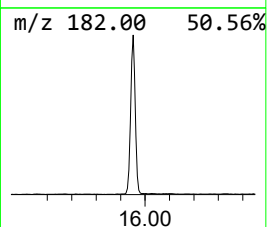
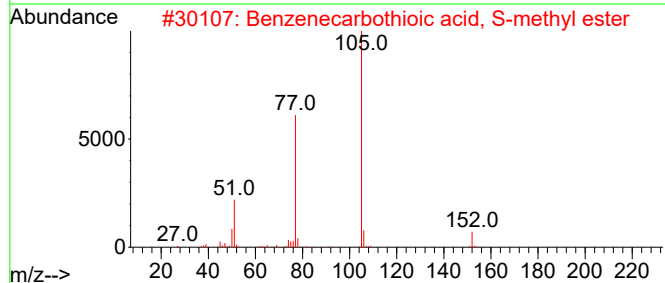
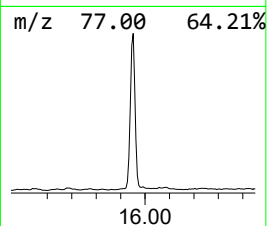
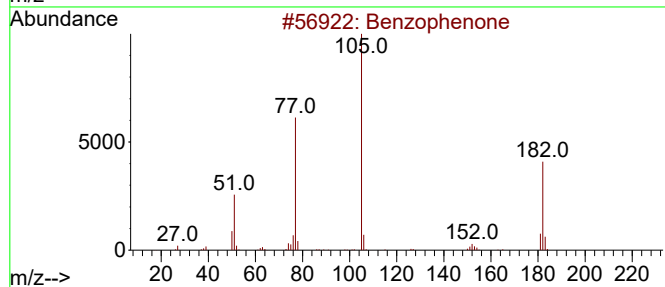
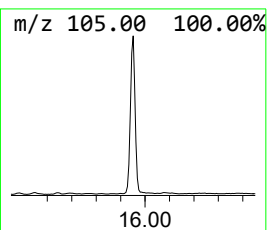
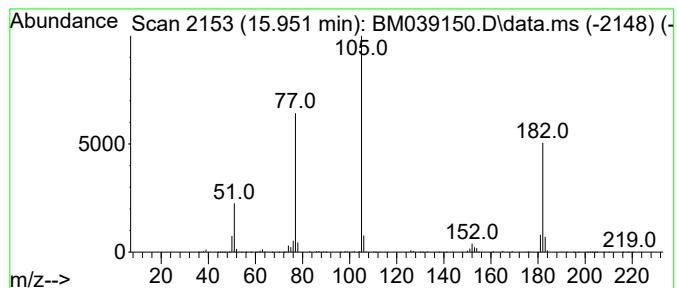
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	15.11 ng	1673900	Acenaphthene-d10	14.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methyl...	152	C8H8OS	005925-68-8	50
3			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Methyl benzilate	242	C15H14O3	000076-89-1	47



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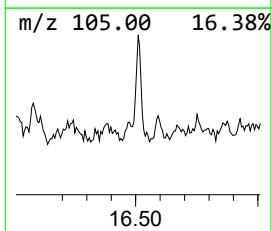
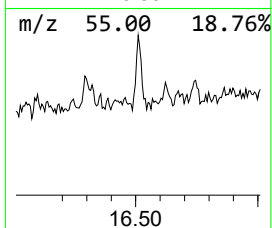
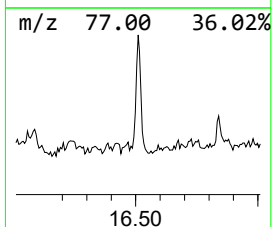
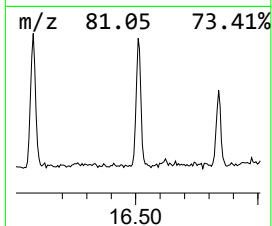
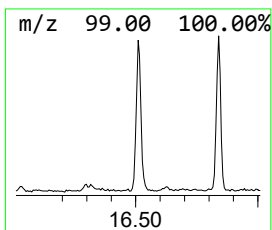
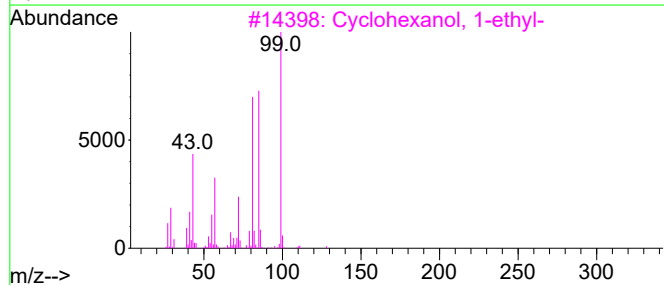
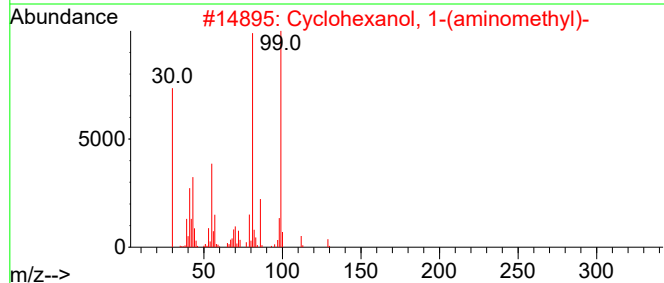
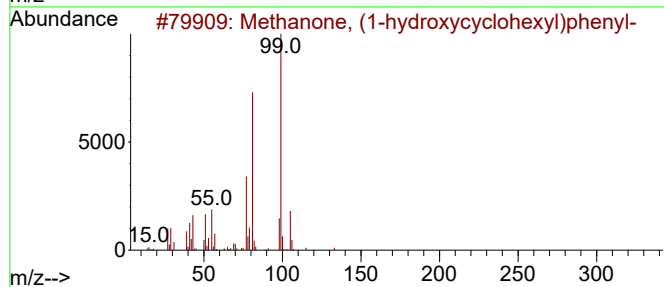
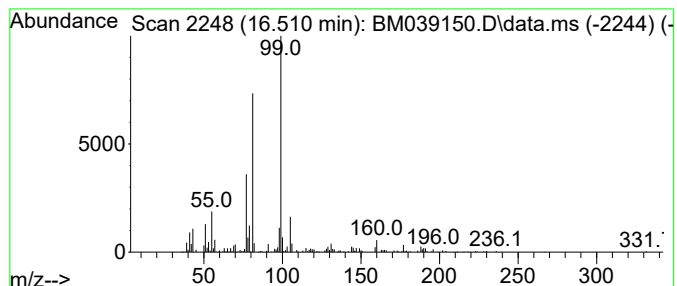
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Peak Number 4 unknown16.510 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.510	2.90 ng	341631	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	49
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	45
3			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	42
4			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	36
5			Androstan-15-one, 5,6-epoxy-2-sp...	346	C21H30O4	299403-62-6	22



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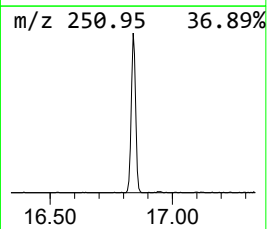
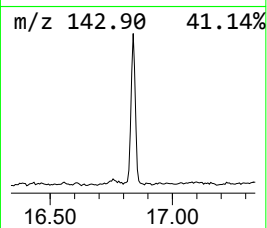
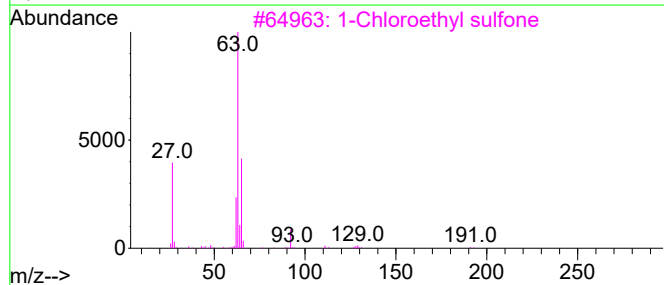
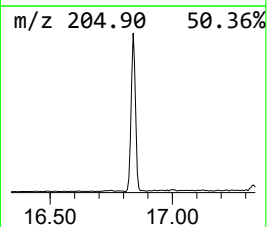
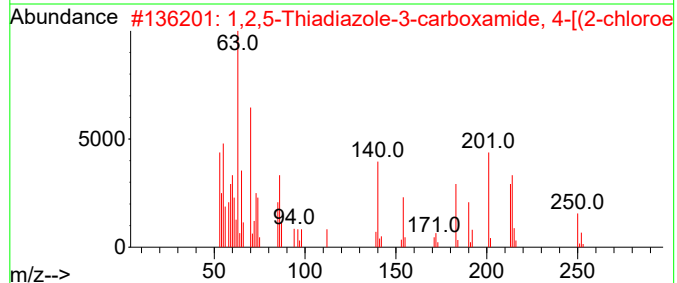
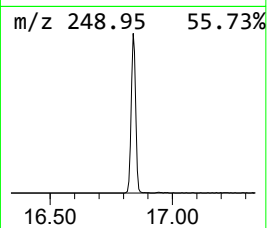
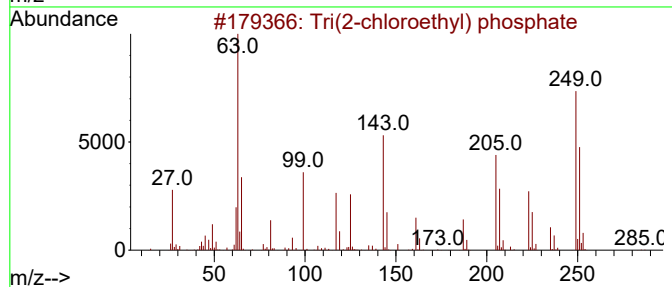
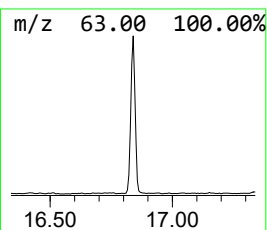
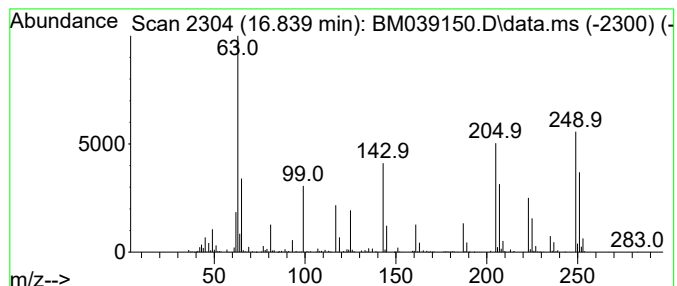
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Peak Number 5 Tri(2-chloroethyl) phosphate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.839	12.20 ng	1434940	Phenanthrene-d10	17.339	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tri(2-chloroethyl) phosphate	284	C6H12Cl3O4P	000115-96-8	95
2	1,2,5-Thiadiazole-3-carboxamide,...	250	C7H11ClN4O2S	147194-45-4	49
3	1-Chloroethyl sulfone	190	C4H8Cl2O2S	010038-07-0	47
4	Ethene, (2-chloroethoxy)-	106	C4H7ClO	000110-75-8	47
5	Oxalyl chloride	126	C2Cl2O2	000079-37-8	43



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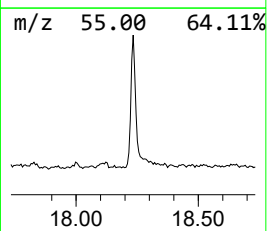
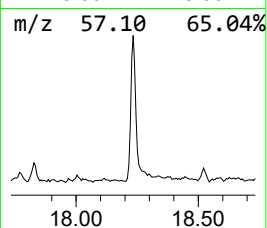
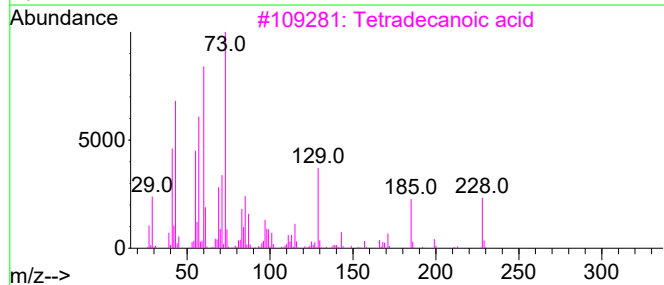
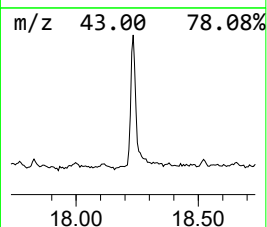
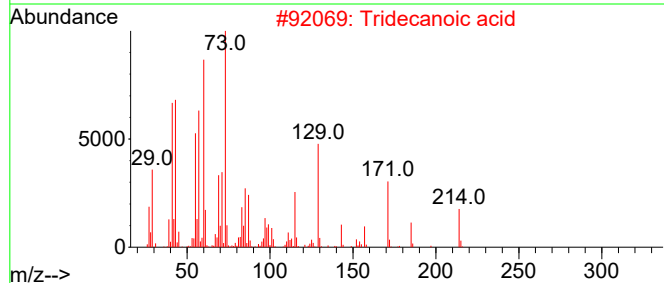
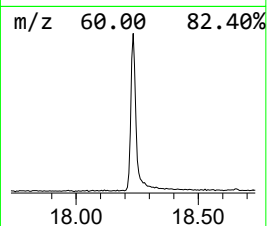
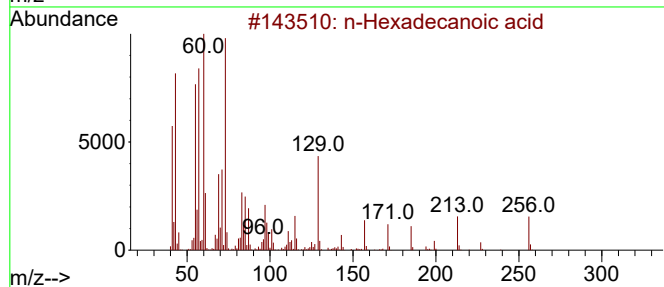
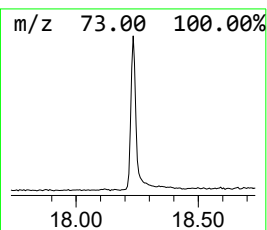
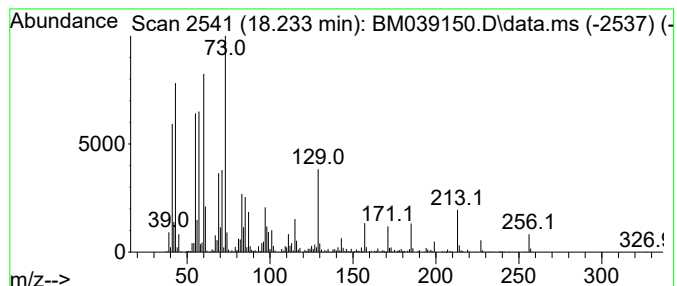
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	12.05 ng	1417540	Phenanthrene-d10	17.339

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	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039150.D
Acq On : 24 Mar 2023 20:22
Operator : CG/JU
Sample : 02069-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-4

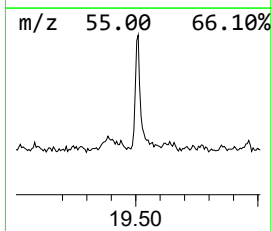
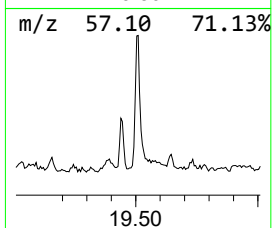
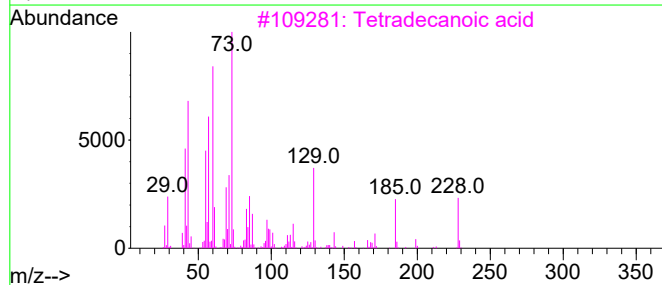
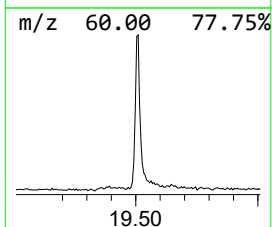
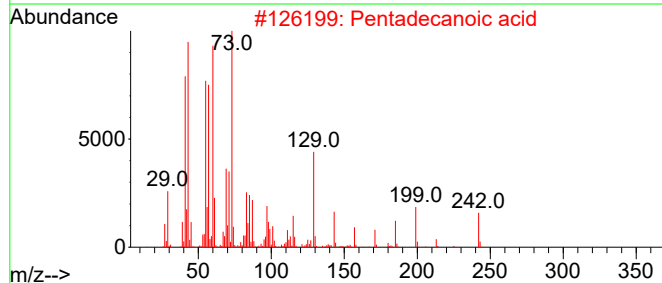
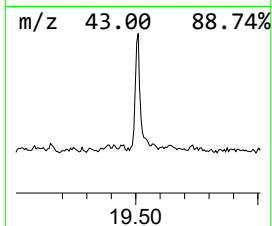
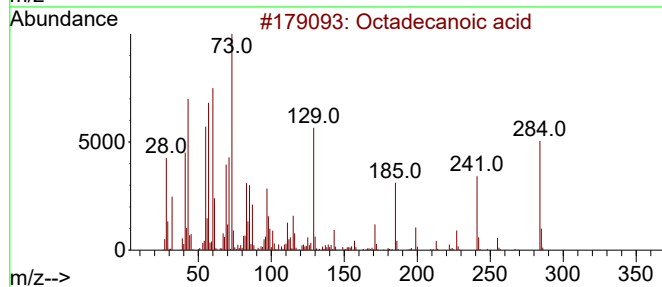
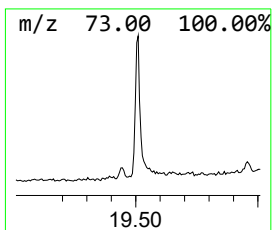
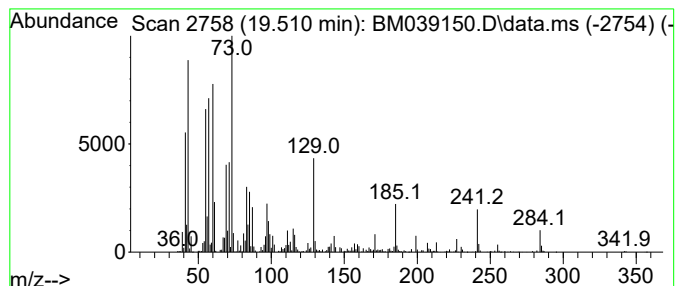
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	5.67 ng	736193	Chrysene-d12	21.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039150.D
Acq On : 24 Mar 2023 20:22
Operator : CG/JU
Sample : 02069-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-4

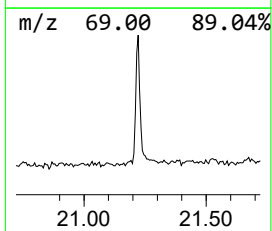
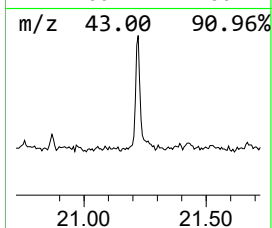
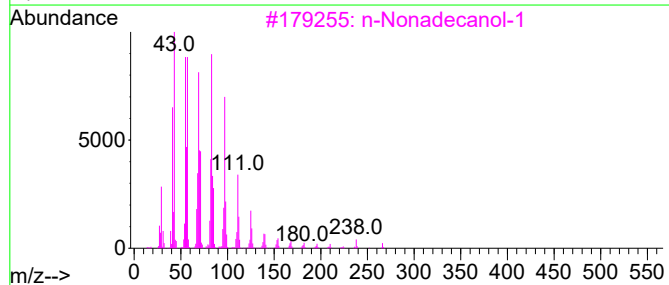
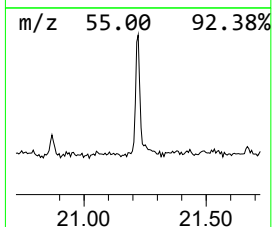
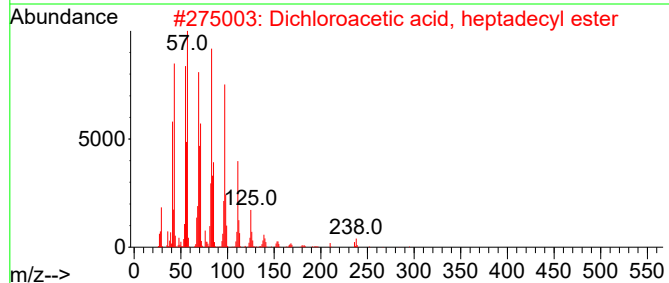
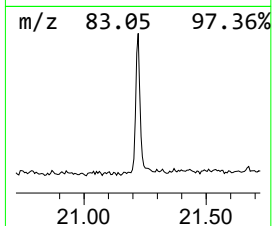
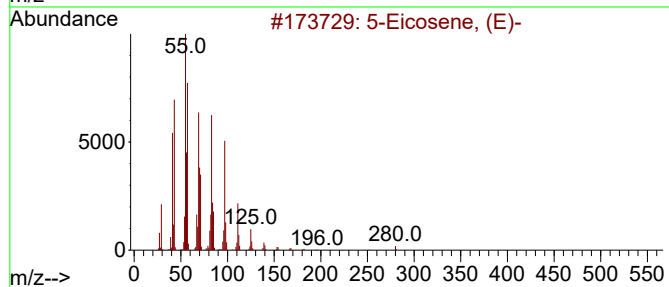
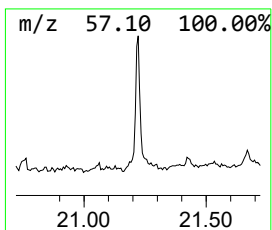
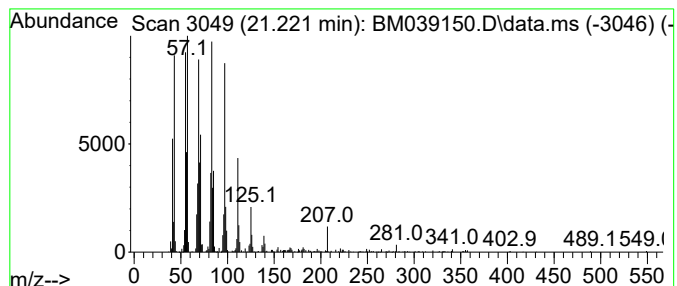
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	3.80 ng	492871	Chrysene-d12	21.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
Data File : BM039150.D
Acq On : 24 Mar 2023 20:22
Operator : CG/JU
Sample : 02069-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
API-3-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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-...	5.040	15.9	ng	1033240	1	7.952	1300740	20.0
unknown15.545	15.545	3.5	ng	386218	3	14.592	2215730	20.0
Benzophenone	15.951	15.1	ng	1673900	3	14.592	2215730	20.0
unknown16.510	16.510	2.9	ng	341631	4	17.339	2352200	20.0
Tri(2-chloroeth...	16.839	12.2	ng	1434940	4	17.339	2352200	20.0
n-Hexadecanoic ...	18.233	12.1	ng	1417540	4	17.339	2352200	20.0
Octadecanoic acid	19.510	5.7	ng	736193	5	21.515	2595010	20.0
5-Eicosene, (E)-	21.221	3.8	ng	492871	5	21.515	2595010	20.0