

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
 Data File : BF134513.D
 Acq On : 27 Jul 2023 19:22
 Operator : CG\JU
 Sample : 03706-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-P20A

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-BF072423.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134513.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.463	570	574	597	rBV	2079865	2000100	100.00%	17.172%
2	6.469	741	745	772	rBV	1713756	1604161	80.20%	13.773%
3	6.822	802	805	811	rBV	519680	481410	24.07%	4.133%
4	6.875	811	814	826	rVB	46593	58185	2.91%	0.500%
5	7.387	897	901	913	rBV	1034631	993238	49.66%	8.528%
6	8.104	1019	1023	1034	rVB	615115	506066	25.30%	4.345%
7	9.181	1202	1206	1209	rBV	1658850	1324420	66.22%	11.371%
8	9.292	1222	1225	1228	rBV	24876	20292	1.01%	0.174%
9	9.863	1318	1322	1325	rBV	552013	474482	23.72%	4.074%
10	10.657	1453	1457	1466	rBV	1097523	953324	47.66%	8.185%
11	11.357	1572	1576	1582	rBV	590634	486670	24.33%	4.178%
12	11.880	1663	1665	1675	rVB2	215084	227856	11.39%	1.956%
13	12.674	1797	1800	1809	rBV3	37413	48768	2.44%	0.419%
14	12.951	1842	1847	1850	rBV	1309821	1196928	59.84%	10.276%
15	13.398	1919	1923	1929	rBV9	10200	23054	1.15%	0.198%
16	13.857	1997	2001	2008	rBV2	122414	226780	11.34%	1.947%
17	14.016	2024	2028	2032	rVB	584584	486327	24.32%	4.175%
18	14.292	2072	2075	2077	rBV4	22191	28148	1.41%	0.242%
19	15.127	2215	2217	2221	rVB	27684	29420	1.47%	0.253%
20	15.515	2278	2283	2291	rBV	226741	300125	15.01%	2.577%
21	17.051	2541	2544	2547	rVB4	29078	33754	1.69%	0.290%
22	17.768	2663	2666	2669	rBV5	24459	34132	1.71%	0.293%
23	17.804	2669	2672	2676	rBV6	24700	38375	1.92%	0.329%
24	18.327	2757	2761	2763	rBV4	23344	38844	1.94%	0.334%
25	18.404	2771	2774	2777	rBV5	22537	32507	1.63%	0.279%

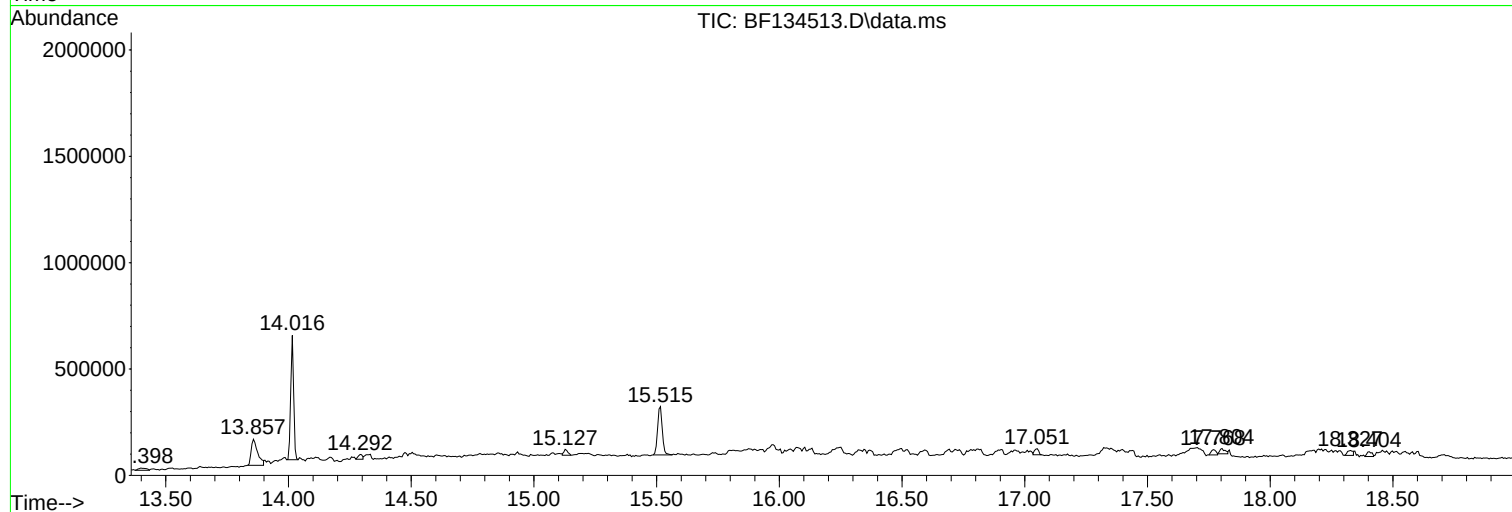
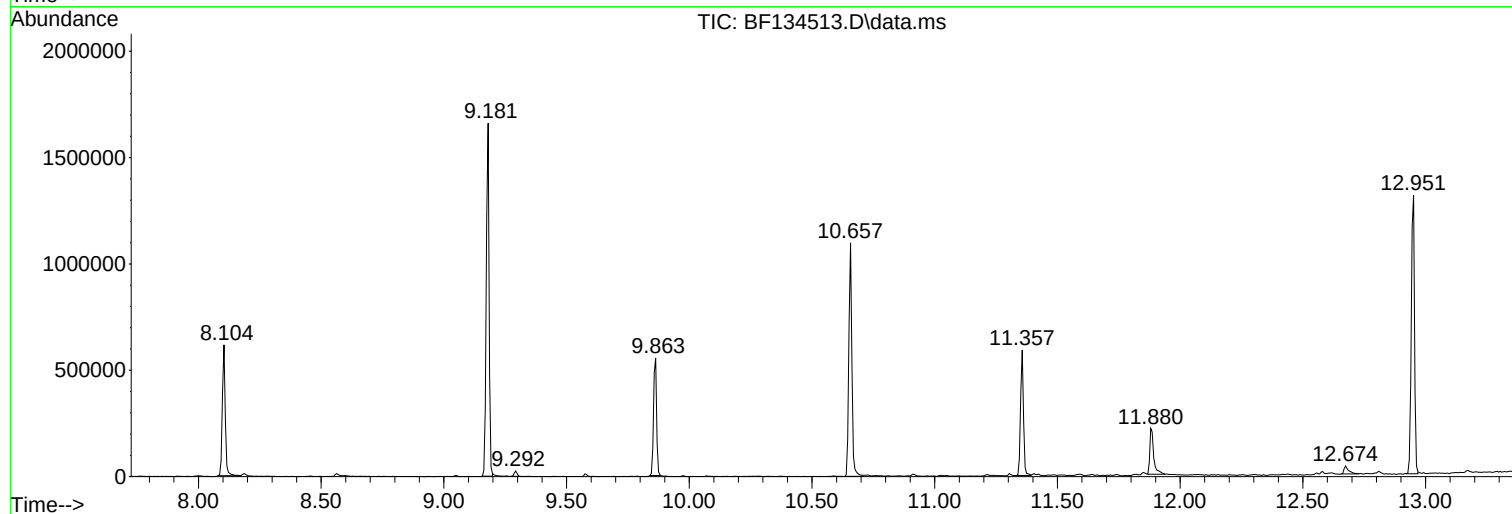
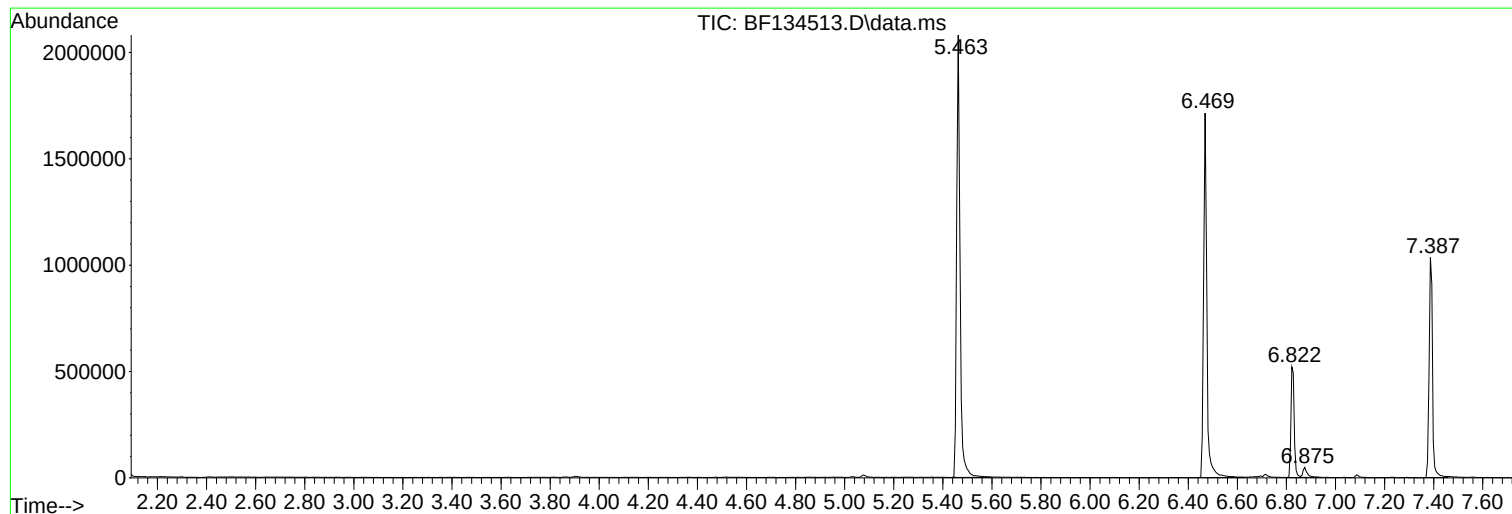
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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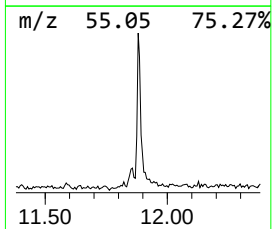
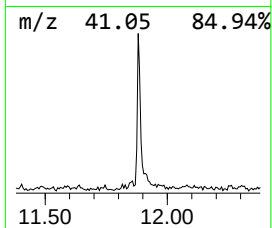
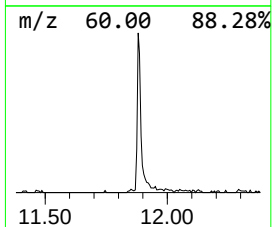
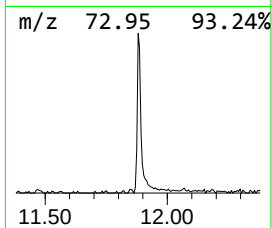
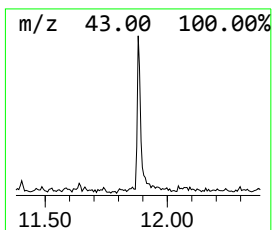
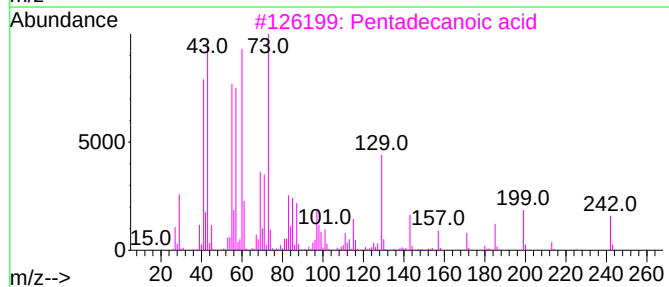
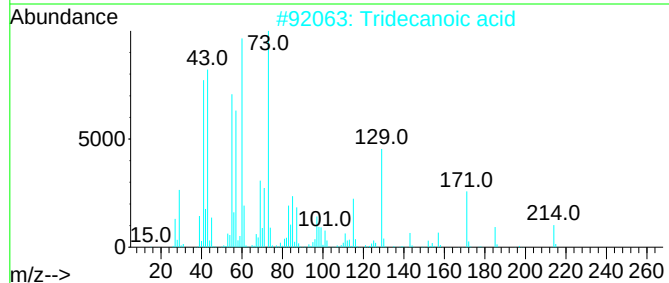
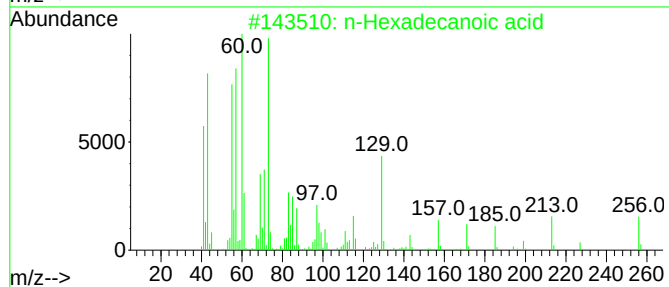
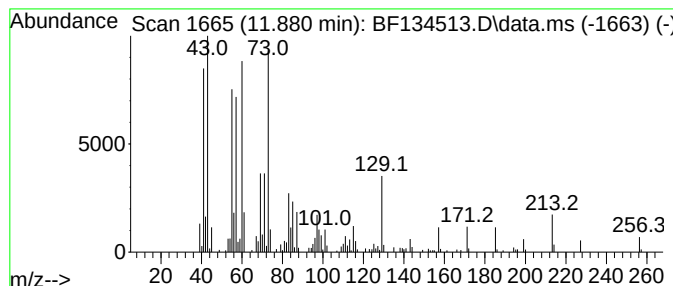
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	9.36 ng	227856	Phenanthrene-d10	11.357

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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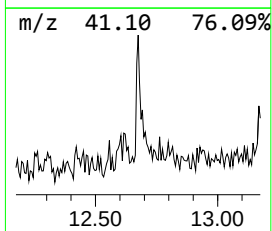
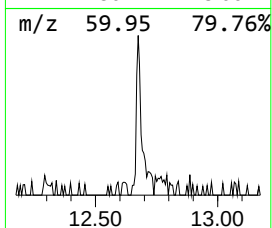
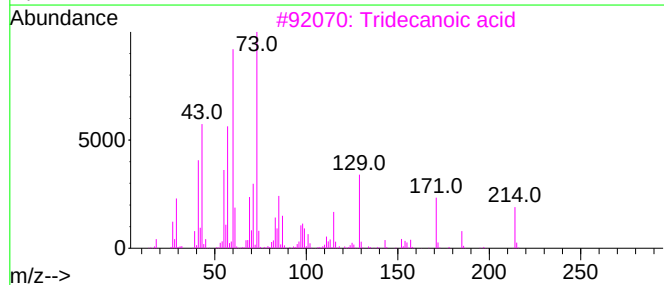
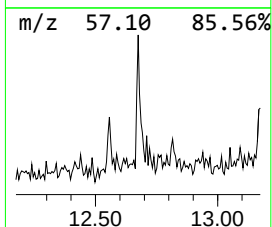
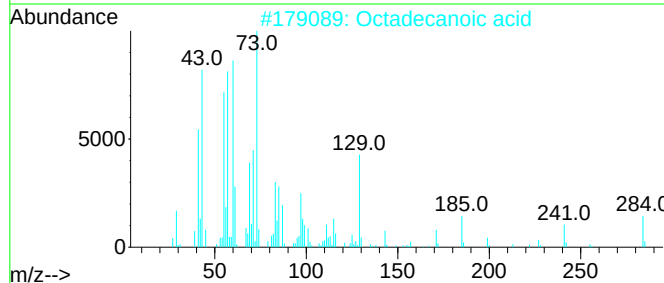
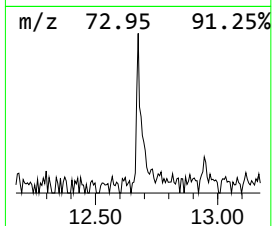
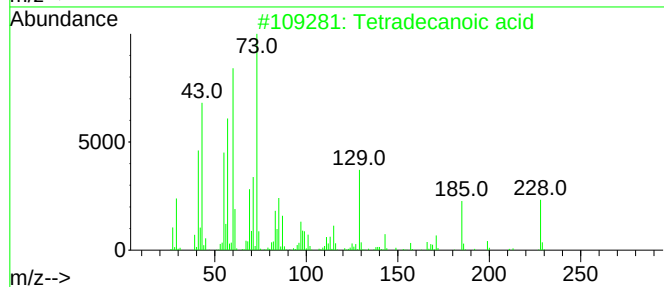
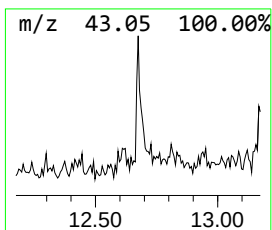
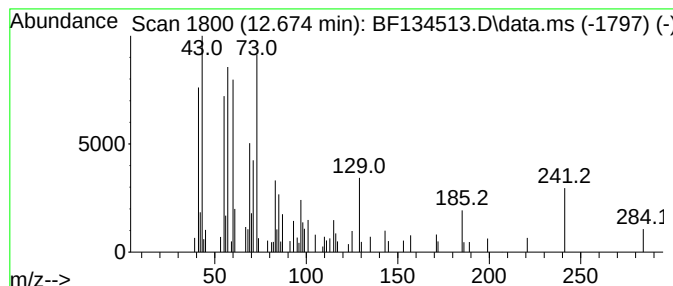
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.675	2.00 ng	48768	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2			Octadecanoic acid	284	C18H36O2	000057-11-4	72
3			Tridecanoic acid	214	C13H26O2	000638-53-9	58
4			Undecanoic acid	186	C11H22O2	000112-37-8	53
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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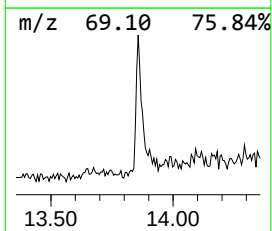
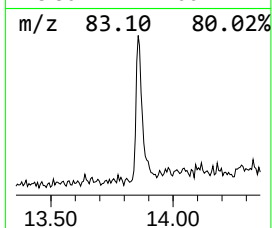
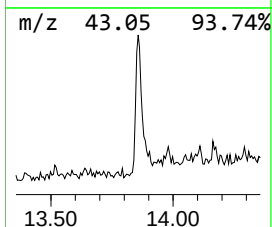
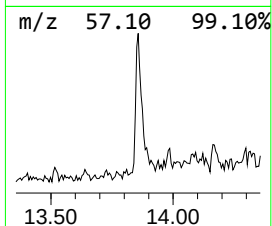
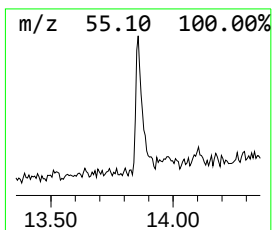
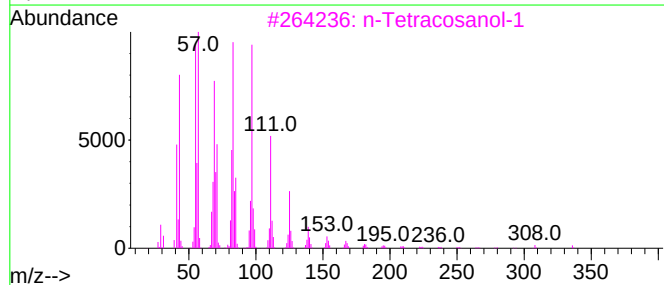
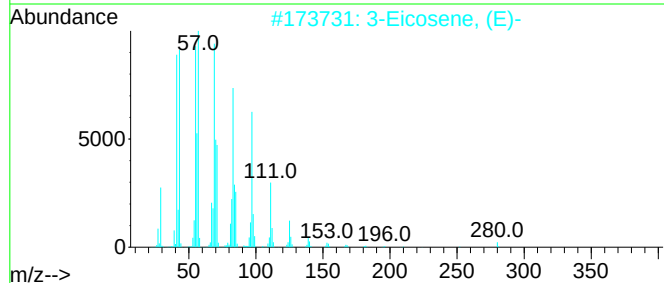
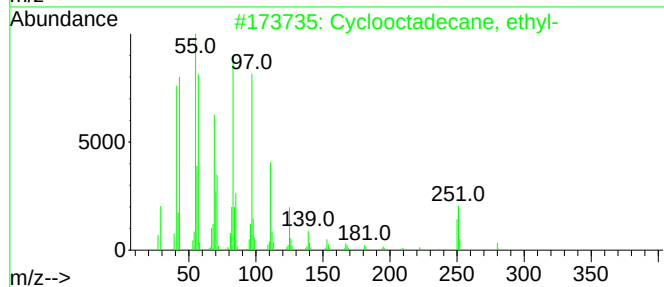
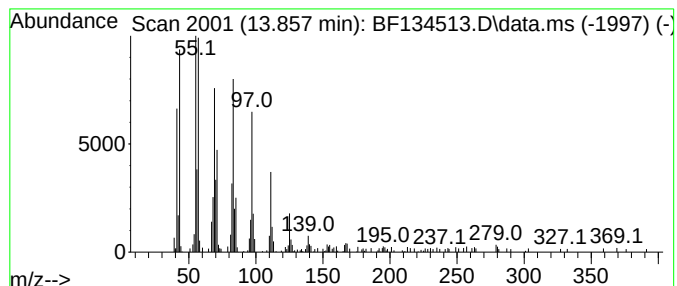
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Peak Number 3 Cyclooctadecane, ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	9.33 ng	226780	Chrysene-d12	14.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	96
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4		Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	95
5		Pentacos-1-ene	350	C25H50	016980-85-1	94



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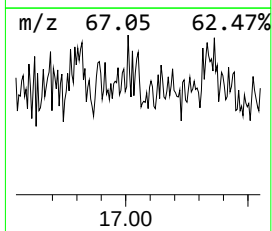
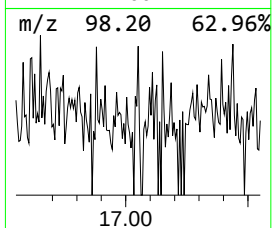
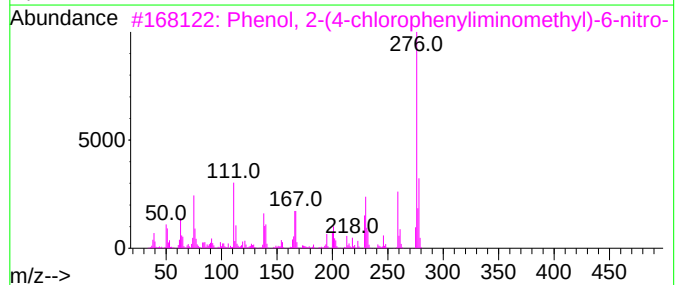
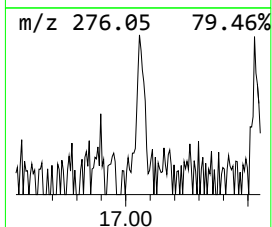
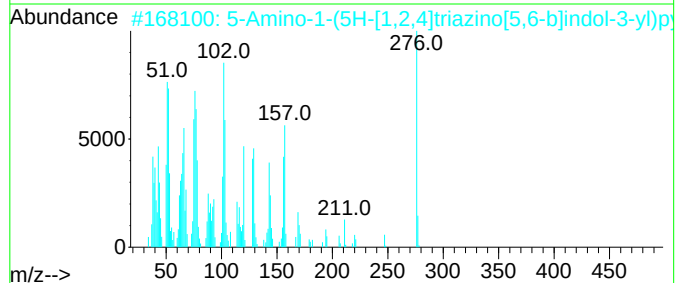
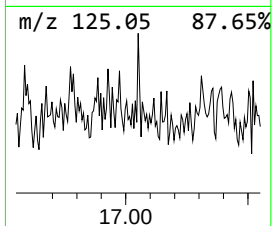
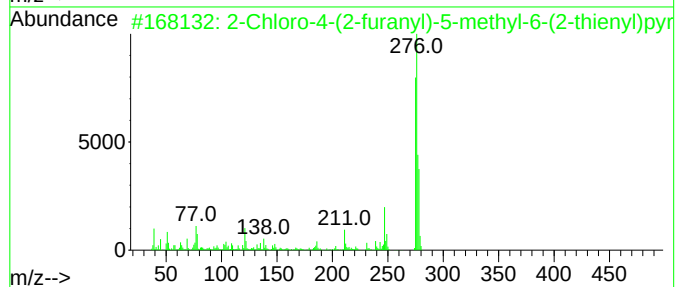
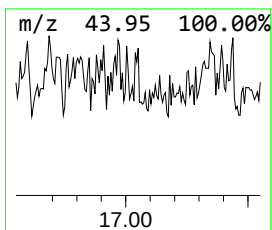
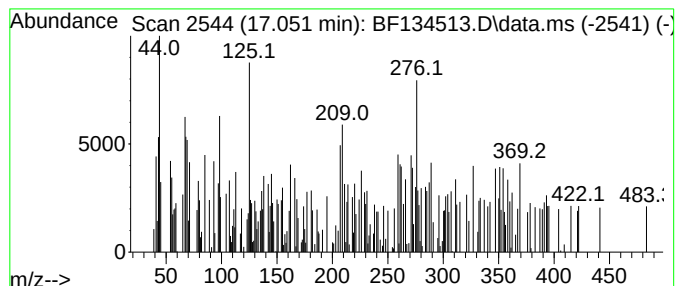
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown17.051 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.051	2.25 ng	33754	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-4-(2-furanyl)-5-methyl-...	276	C13H9ClN2O5	131022-80-5	15
2	5-Amino-1-(5H-[1,2,4]triazino[5,...	276	C13H8N8	073718-31-7	11
3	Phenol, 2-(4-chlorophenyliminome...	276	C13H9ClN2O3	1000262-90-3	11
4	5H-Thiazolo[3,2-a]pyrimidin-5-on...	276	C13H9ClN2O5	023429-91-6	11
5	N-(3-Amino-4-fluorophenyl)methan...	276	C10H17FN2O2SSi	1000511-95-9	11



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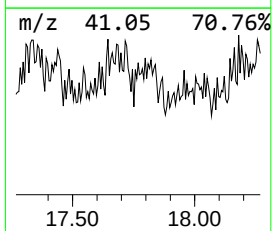
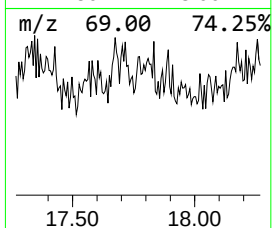
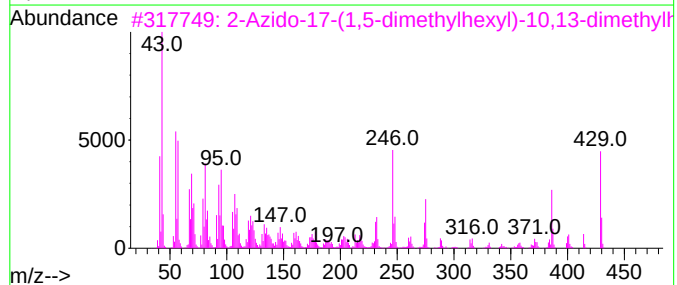
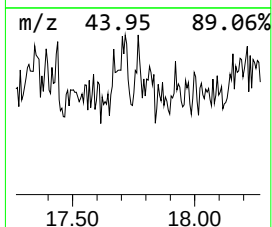
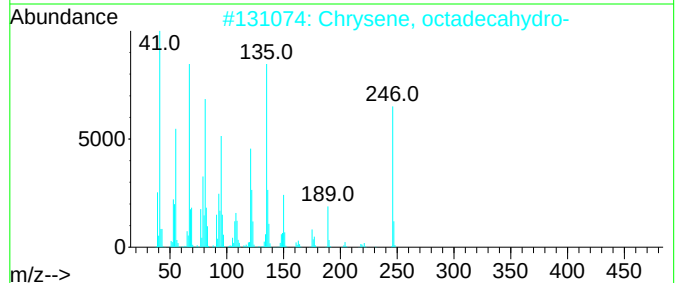
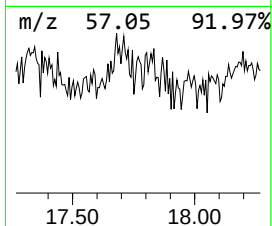
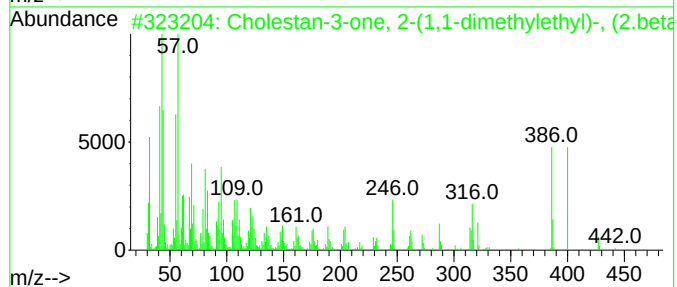
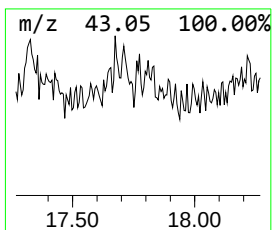
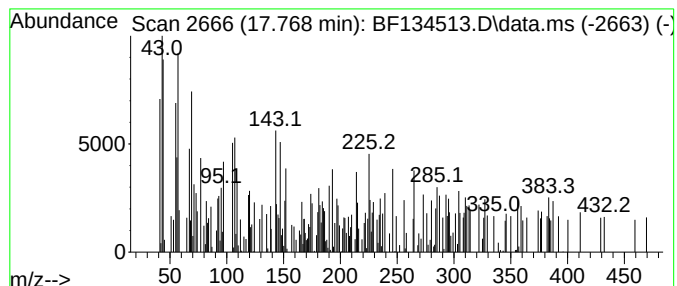
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Peak Number 5 unknown17.768 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.768	2.27 ng	34132	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-one, 2-(1,1-dimethyl...	442	C31H54O	055162-57-7	16
2			Chrysene, octadecahydro-	246	C18H30	002090-14-4	11
3			2-Azido-17-(1,5-dimethylhexyl)-1...	429	C27H47N3O	1000210-24-9	10
4			Acetamide, N-[4-(2-hydroxybenzyl)...	246	C11H10N4O3	1000277-50-1	10
5			N-(2-Methyl-4-nitro-5-pyrrolidin...	263	C13H17N3O3	1010296-76-3	10



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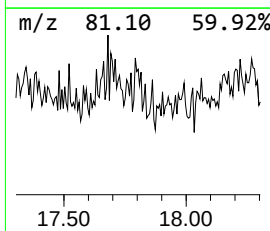
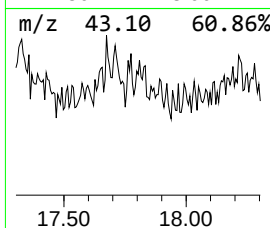
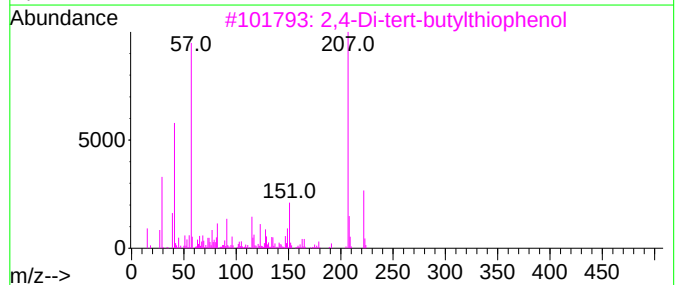
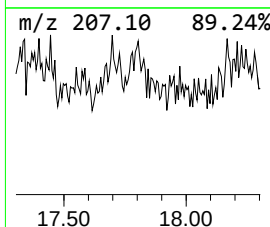
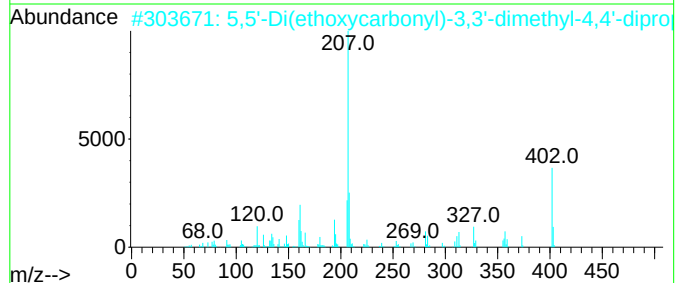
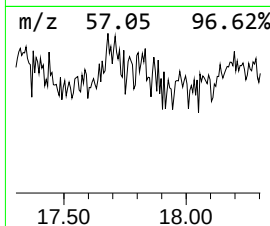
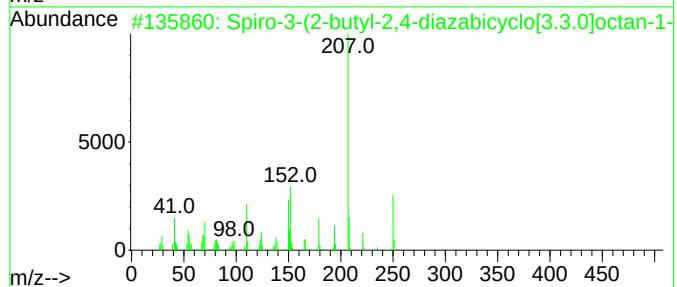
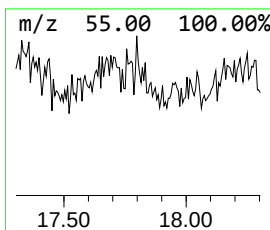
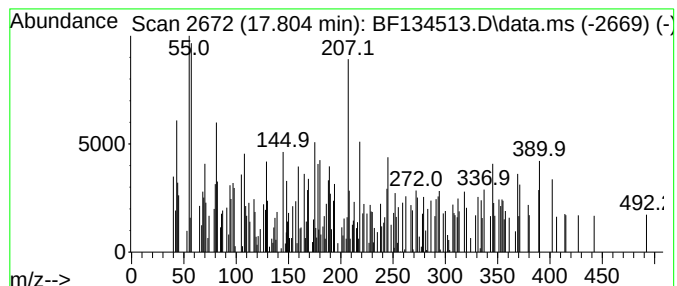
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.804 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.804	2.56 ng	38375	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro-3-(2-butyl-2,4-diazabicycl...	250	C15H26N2O	1000194-74-4	25
2			5,5'-Di(ethoxycarbonyl)-3,3'-dim...	402	C23H34N2O4	102586-97-0	22
3			2,4-Di-tert-butylthiophenol	222	C14H22S	019728-43-9	15
4			Pyrazolo[5,1-c][1,2,4]triazine-3...	279	C11H13N5O4	1000302-77-3	15
5			Mycophenolic acid IV	388	C22H28O6	074838-16-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134513.D
Acq On : 27 Jul 2023 19:22
Operator : CG\JU
Sample : 03706-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P20A

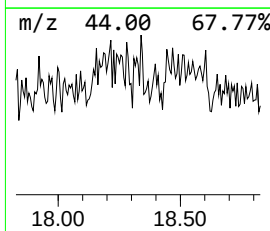
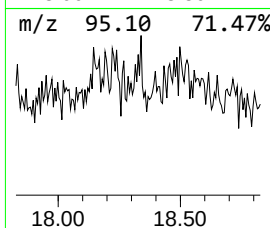
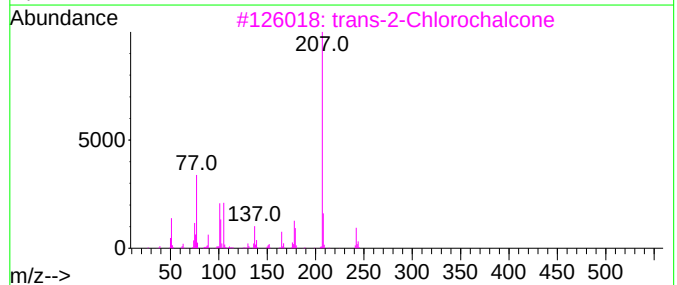
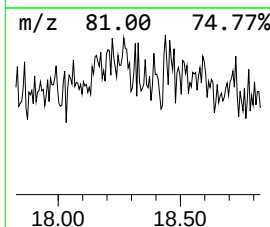
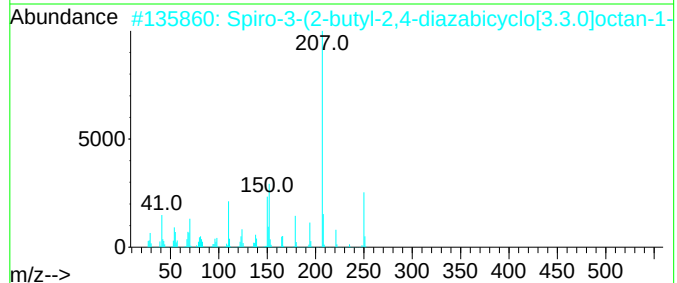
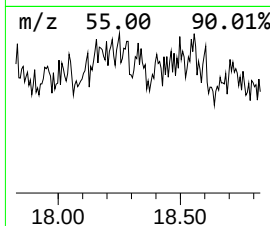
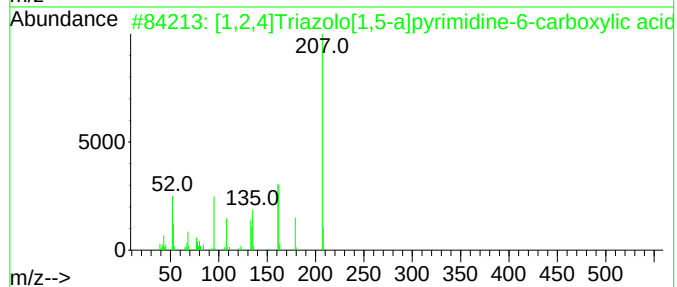
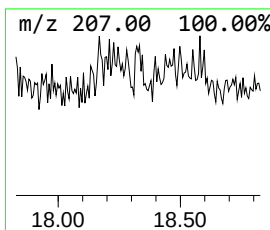
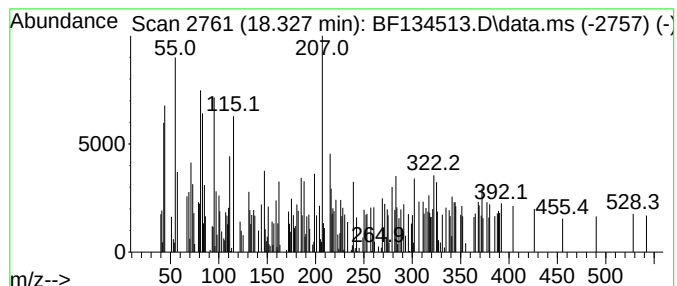
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown18.327 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.327	2.59 ng	38844	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,2,4]Triazolo[1,5-a]pyrimidine...	207	C8H9N5O2	092673-40-0	30
2			Spiro-3-(2-butyl-2,4-diazabicycl...	250	C15H26N2O	1000194-74-4	30
3			trans-2-Chlorochalcone	242	C15H11ClO	022966-11-6	25
4			3,6-Dinitro-1H-indole	207	C8H5N3O4	004771-15-7	25
5			2-Nitro-4-(trifluoromethyl)phenol	207	C7H4F3NO3	000400-99-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134513.D
Acq On : 27 Jul 2023 19:22
Operator : CG\JU
Sample : 03706-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P20A

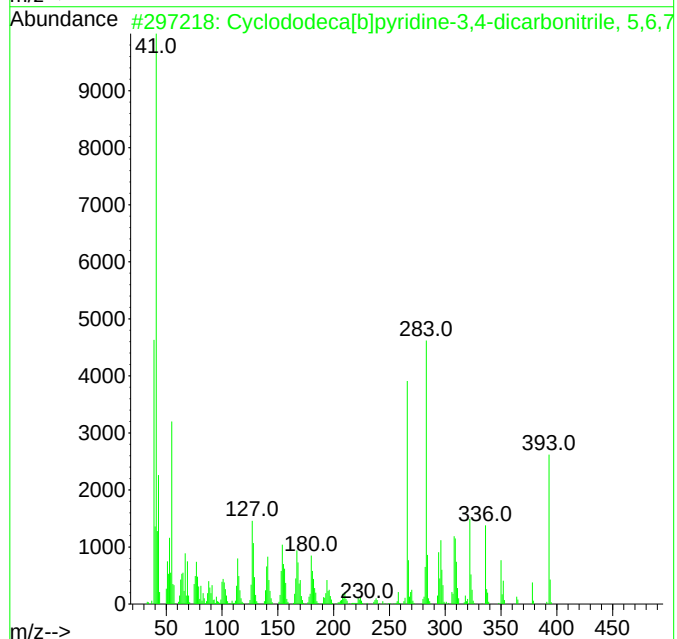
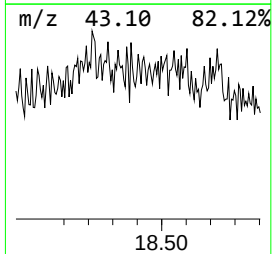
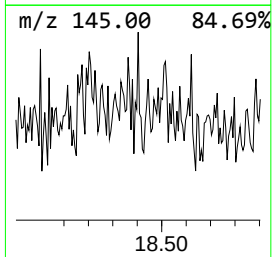
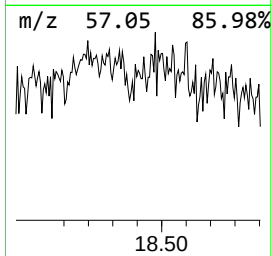
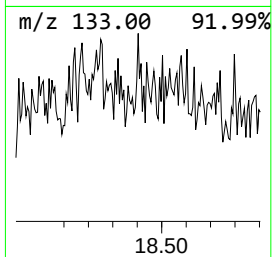
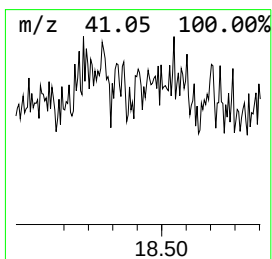
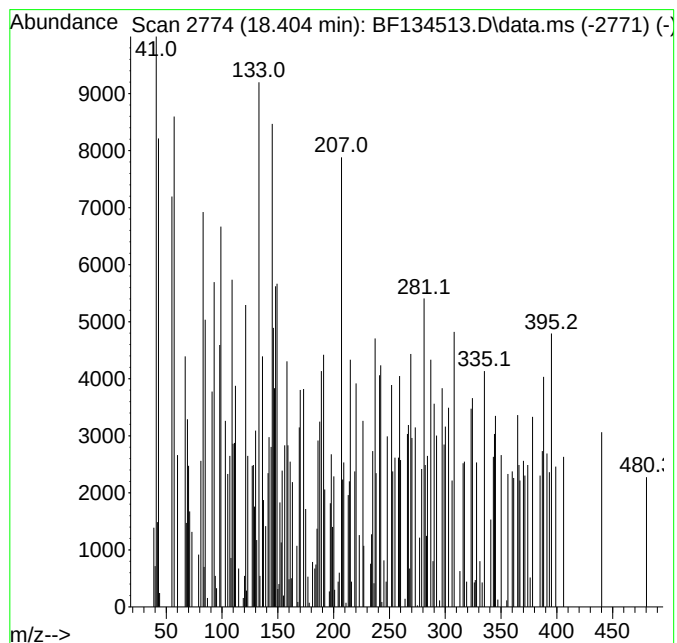
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.404 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.404	2.17 ng	32507	Perylene-d12	15.515

Hit#	of	1	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododeca[b]pyridine-3,4-dicar...	393	C17H20IN3	1000277-20-5	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072723\
Data File : BF134513.D
Acq On : 27 Jul 2023 19:22
Operator : CG\JU
Sample : 03706-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-P20A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.880	9.4	ng	227856	4	11.357	486670	20.0
Tetradecanoic acid	12.675	2.0	ng	48768	4	11.357	486670	20.0
Cyclooctadecane...	13.857	9.3	ng	226780	5	14.016	486327	20.0
unknown17.051	17.051	2.3	ng	33754	6	15.515	300125	20.0
unknown17.768	17.768	2.3	ng	34132	6	15.515	300125	20.0
unknown17.804	17.804	2.6	ng	38375	6	15.515	300125	20.0
unknown18.327	18.327	2.6	ng	38844	6	15.515	300125	20.0
unknown18.404	18.404	2.2	ng	32507	6	15.515	300125	20.0