

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
 Data File : BF123827.D
 Acq On : 5 May 2021 14:56
 Operator : JU/CG
 Sample : M2275-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CRT-020

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-BF042721.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	493	496	503	rVB	71122	89910	1.30%	0.183%
2	5.416	562	566	569	rBV	7436079	6617452	95.99%	13.495%
3	6.434	735	739	751	rVB	6353751	6894167	100.00%	14.059%
4	6.622	768	771	778	rBV2	77057	98055	1.42%	0.200%
5	6.792	796	800	803	rBV	1882502	1419517	20.59%	2.895%
6	7.357	891	896	899	rBV	4790032	4487173	65.09%	9.151%
7	8.080	1015	1019	1022	rBV	2110580	1862583	27.02%	3.798%
8	9.157	1197	1202	1205	rBV	7822746	6642293	96.35%	13.545%
9	9.551	1266	1269	1272	rBV	456978	377466	5.48%	0.770%
10	9.833	1313	1317	1321	rVB	2487829	2003616	29.06%	4.086%
11	10.245	1384	1387	1389	rBV2	98879	86975	1.26%	0.177%
12	10.492	1426	1429	1432	rBV	134481	130691	1.90%	0.267%
13	10.627	1447	1452	1455	rBV	5376221	4715218	68.39%	9.616%
14	10.757	1470	1474	1480	rBV	344270	443330	6.43%	0.904%
15	11.227	1551	1554	1557	rVB	272587	271868	3.94%	0.554%
16	11.321	1567	1570	1573	rBV	2357676	1980225	28.72%	4.038%
17	11.857	1659	1661	1670	rVB4	304685	322074	4.67%	0.657%
18	12.915	1836	1841	1844	rBV	6457988	5786537	83.93%	11.800%
19	13.827	1992	1996	2009	rVB2	453697	898522	13.03%	1.832%
20	13.968	2016	2020	2023	rBV	1627045	1460885	21.19%	2.979%
21	14.445	2098	2101	2103	rBV	94156	97043	1.41%	0.198%
22	14.468	2103	2105	2114	rVB6	86618	166686	2.42%	0.340%
23	14.821	2163	2165	2170	rVB6	59294	76227	1.11%	0.155%
24	15.080	2206	2209	2214	rBV	238021	250687	3.64%	0.511%
25	15.421	2262	2267	2271	rBV	1066370	1310218	19.00%	2.672%
26	15.456	2271	2273	2277	rVB2	79746	86851	1.26%	0.177%
27	15.886	2342	2346	2352	rVB	220880	328902	4.77%	0.671%
28	17.033	2538	2541	2547	rVB8	79030	132243	1.92%	0.270%

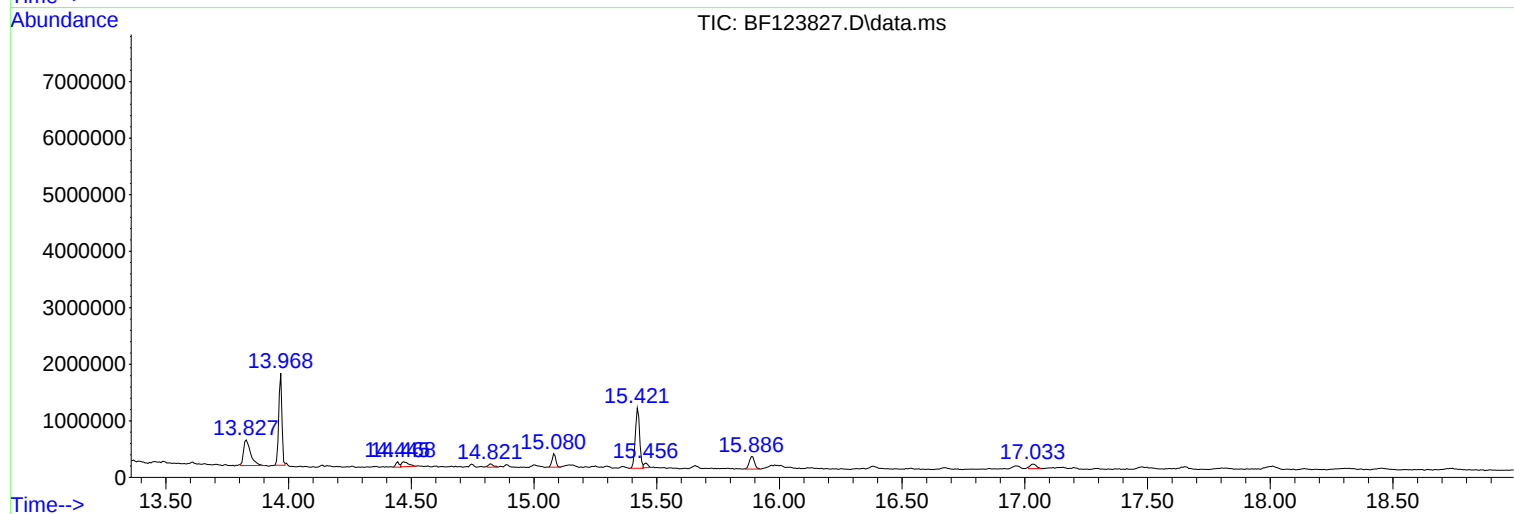
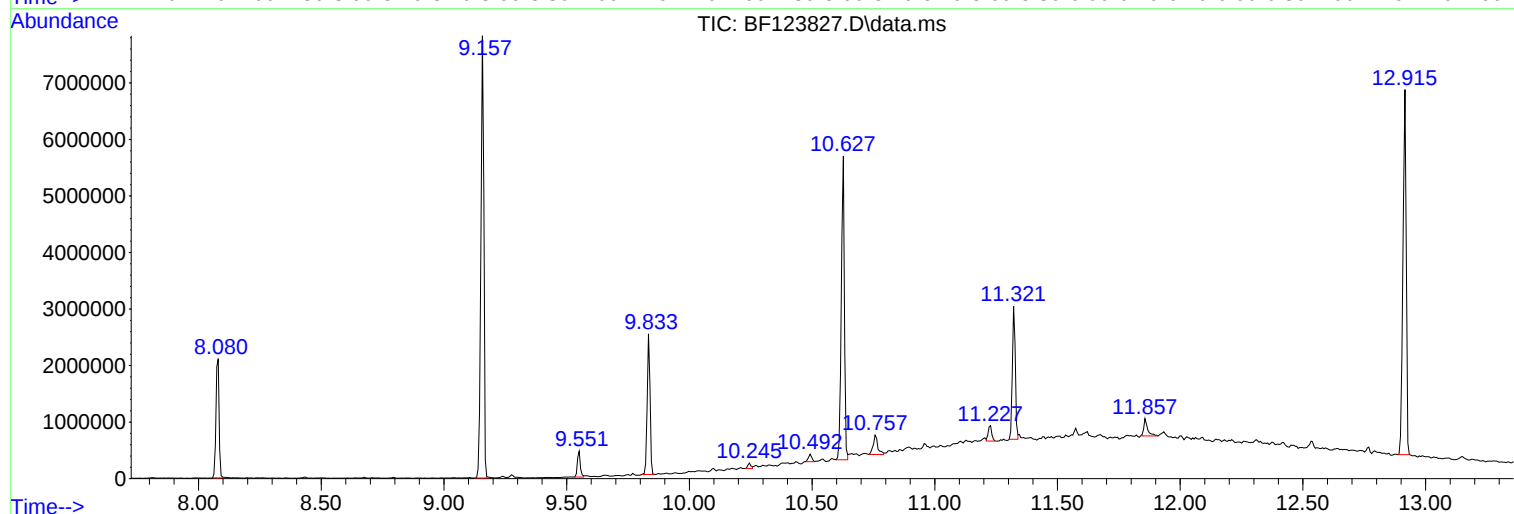
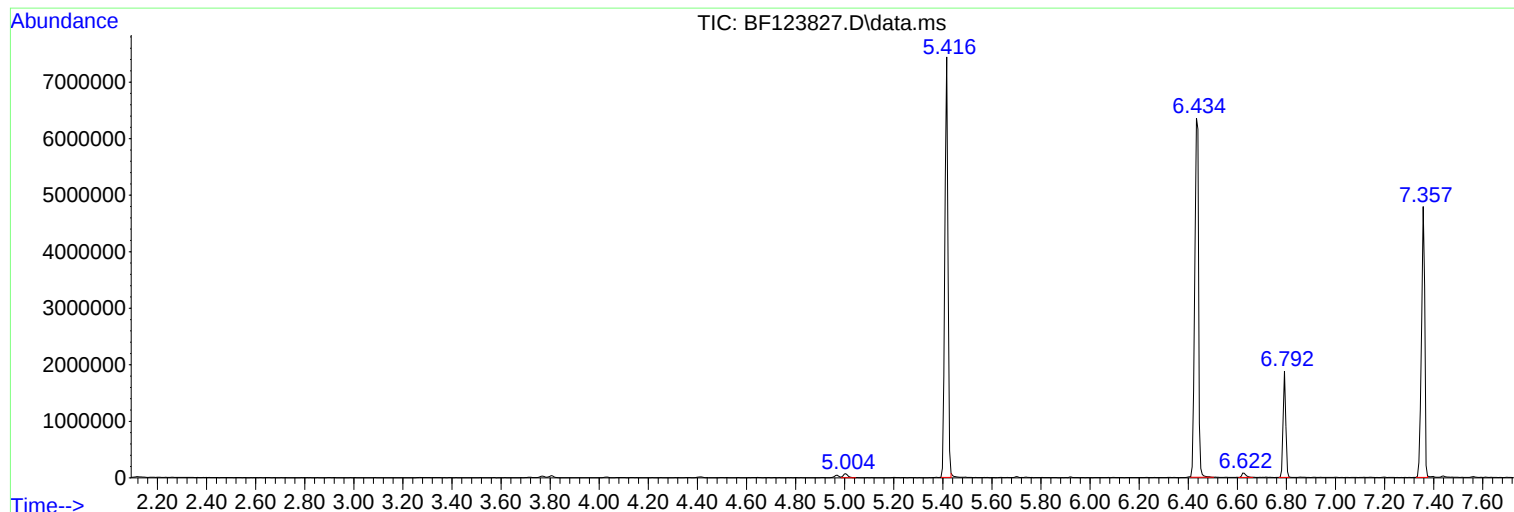
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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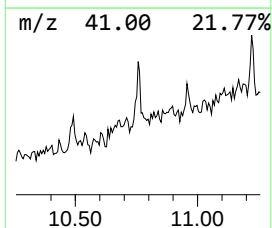
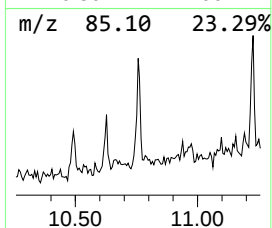
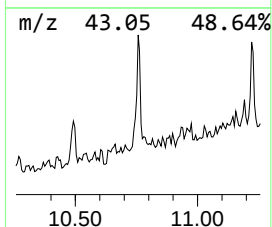
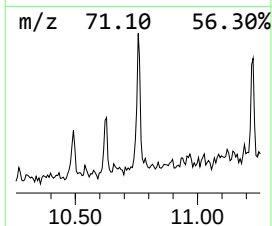
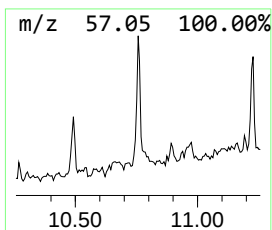
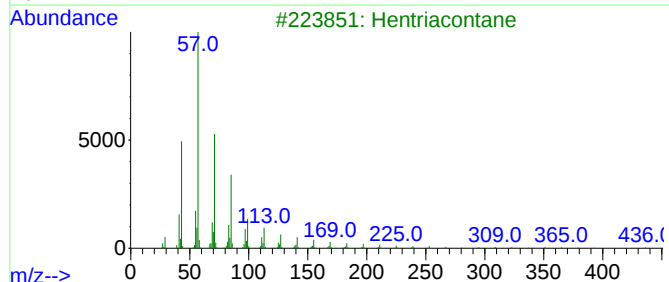
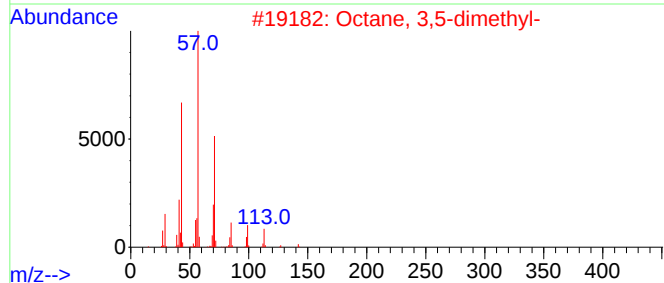
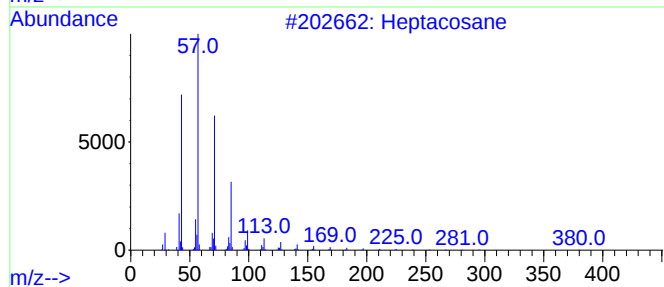
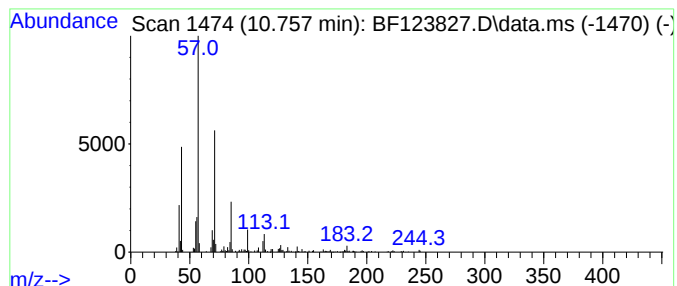
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Octane, 3,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	4.48 ng	443330	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	86
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	80
3			Hentriacontane	437	C31H64	000630-04-6	72
4			Hexadecane	226	C16H34	000544-76-3	64
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	58



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ClientSampled :
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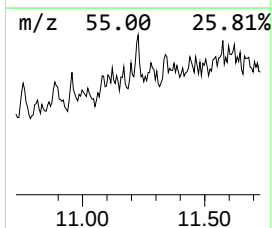
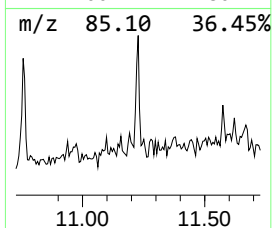
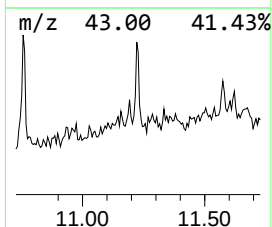
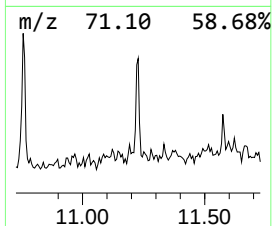
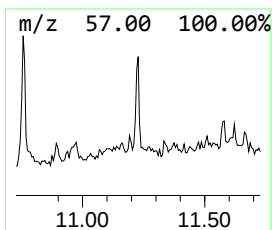
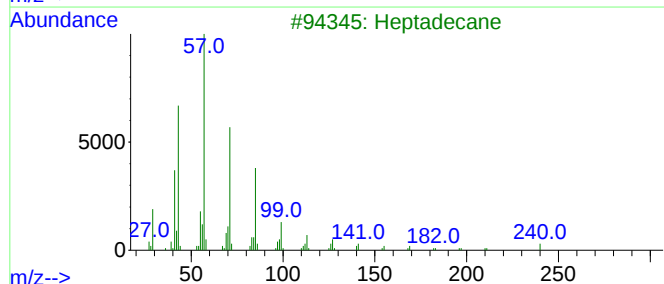
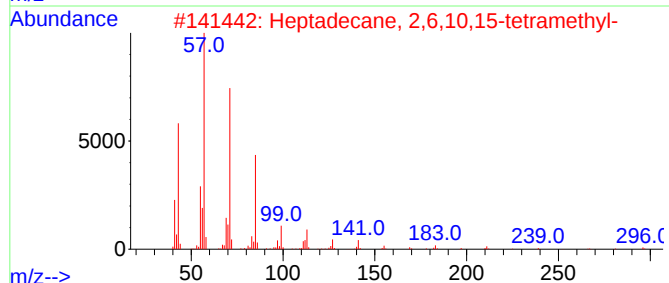
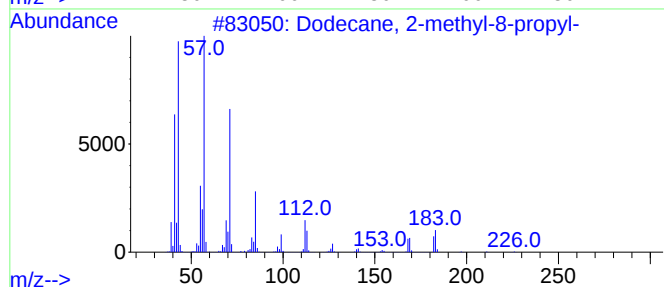
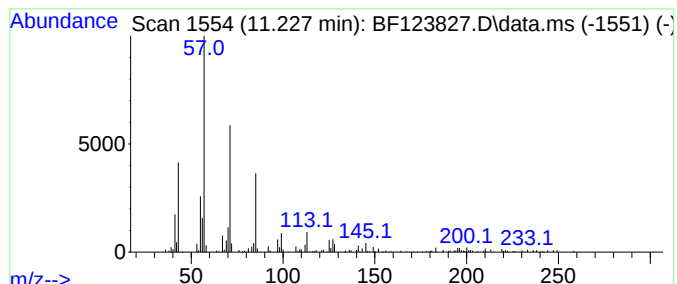
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane, 2-methyl-8-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.227	2.75 ng	271868	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	83
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
3			Heptadecane	240	C17H36	000629-78-7	83
4			Heptacosane	380	C27H56	000593-49-7	80
5			Pentadecane, 7-methyl-	226	C16H34	006165-40-8	76



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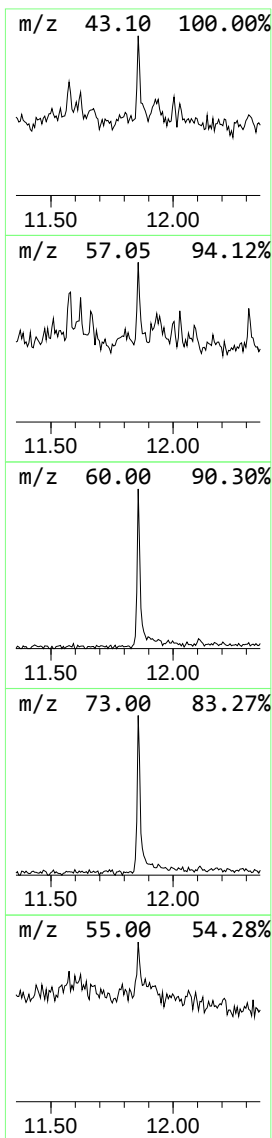
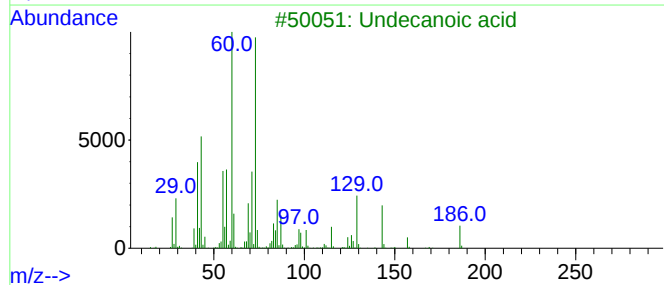
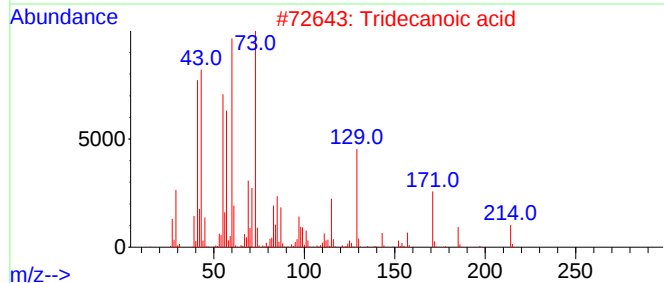
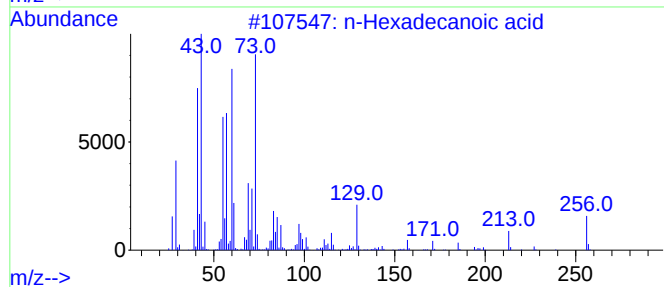
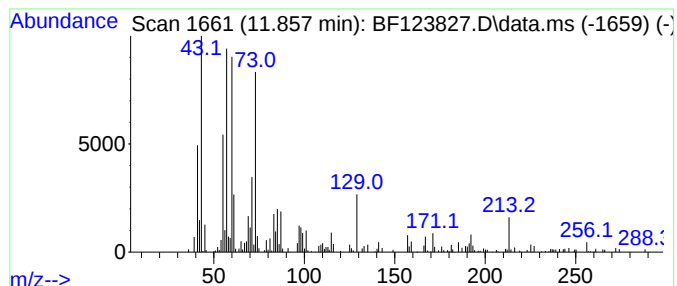
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.857	3.25 ng	322074	Phenanthrene-d10		11.322	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	91
2	Tridecanoic acid		214	C13H26O2	000638-53-9	90
3	Undecanoic acid		186	C11H22O2	000112-37-8	80
4	n-Decanoic acid		172	C10H20O2	000334-48-5	62
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	59



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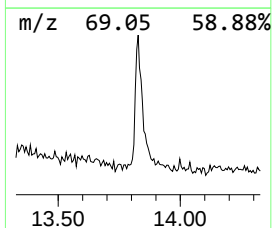
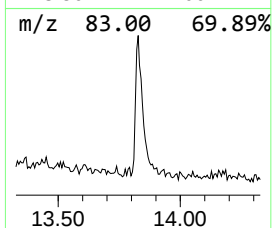
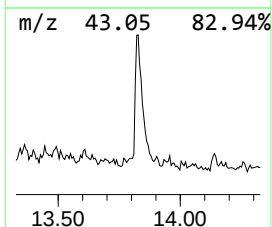
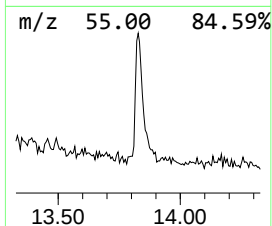
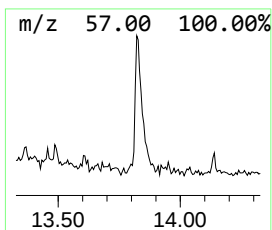
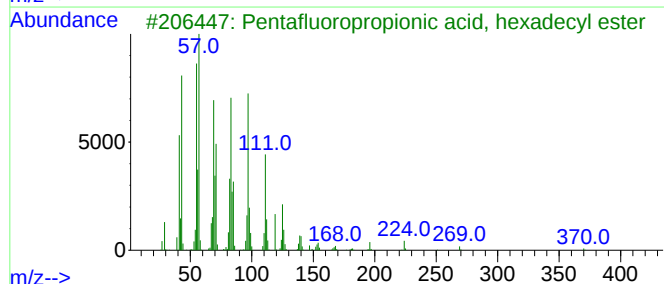
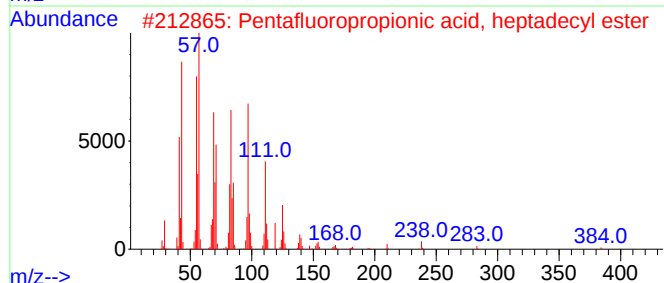
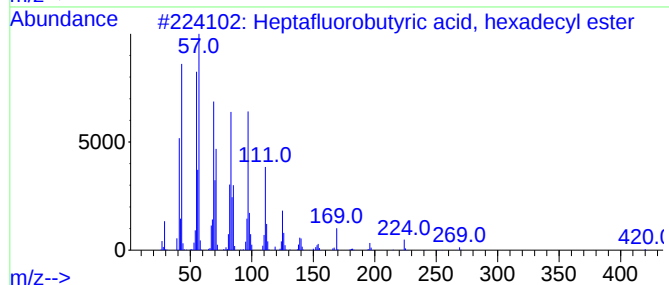
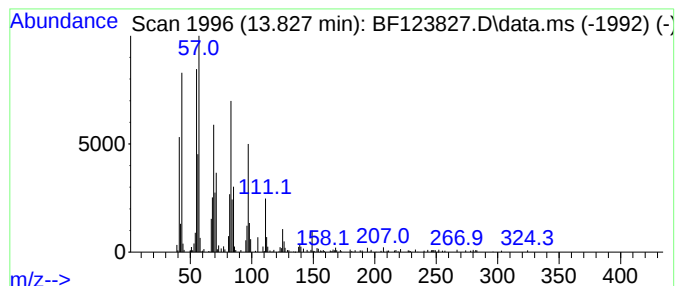
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Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	12.30 ng	898522	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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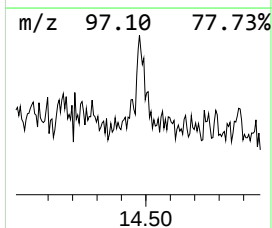
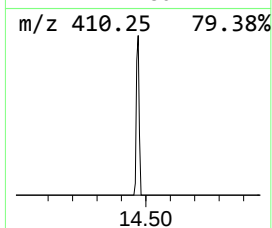
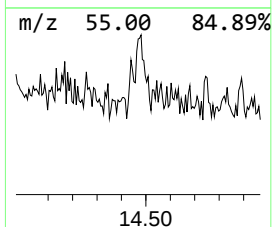
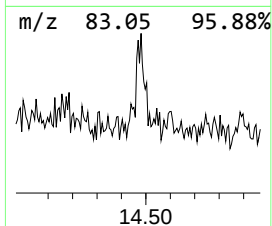
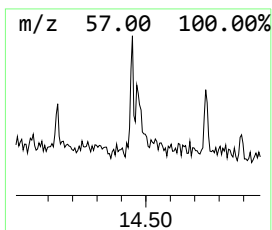
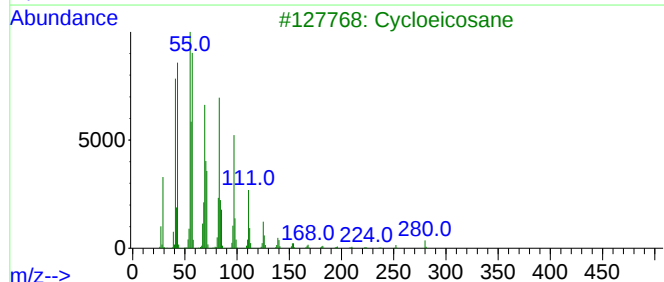
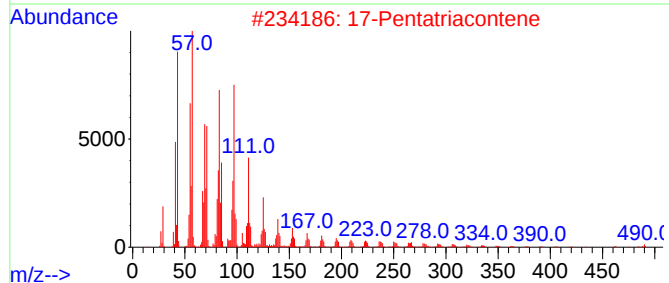
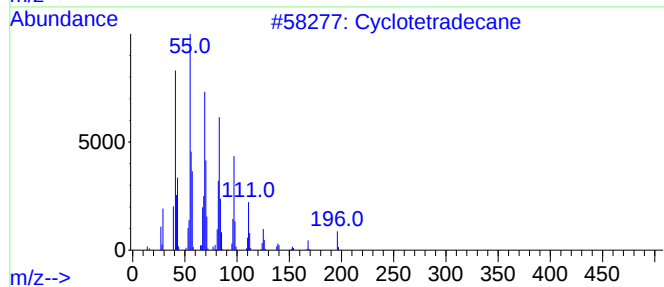
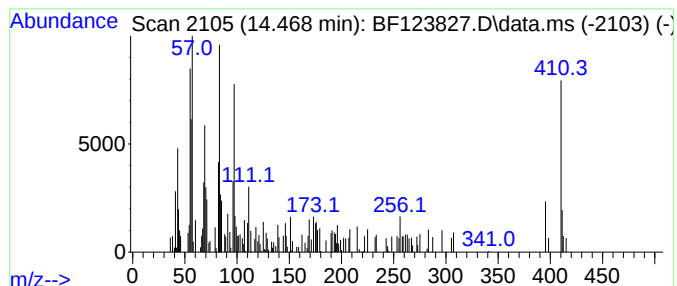
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.468	2.28 ng	166686	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	51
2			17-Pentatriacontene	491	C35H70	006971-40-0	45
3			Cycloeicosane	280	C20H40	000296-56-0	43
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	38
5			Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	38



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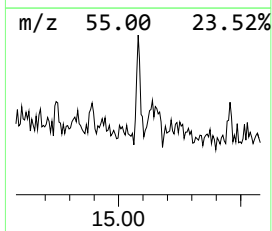
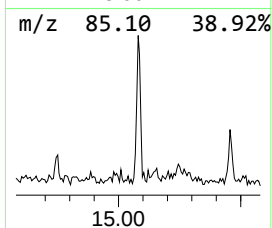
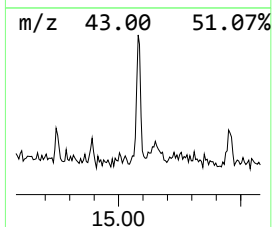
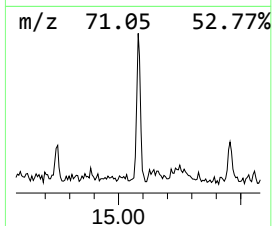
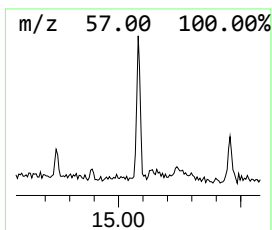
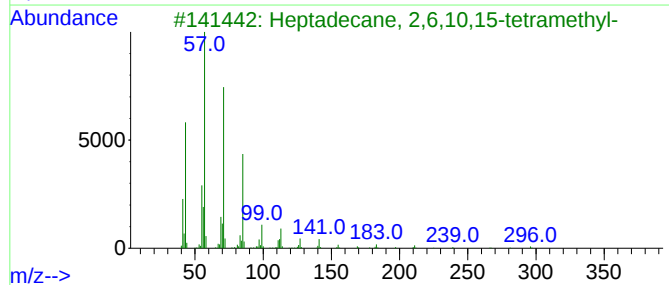
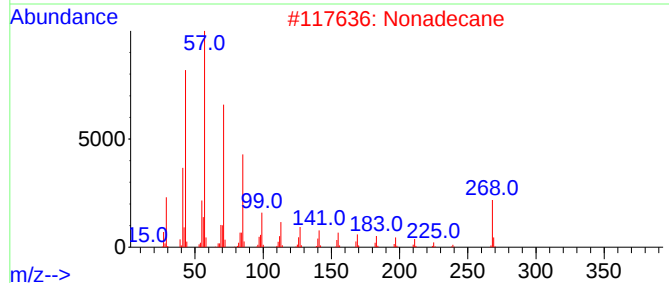
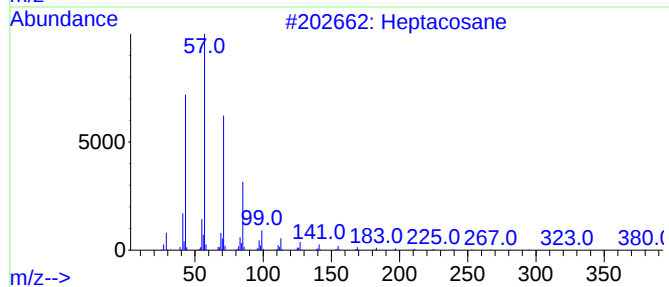
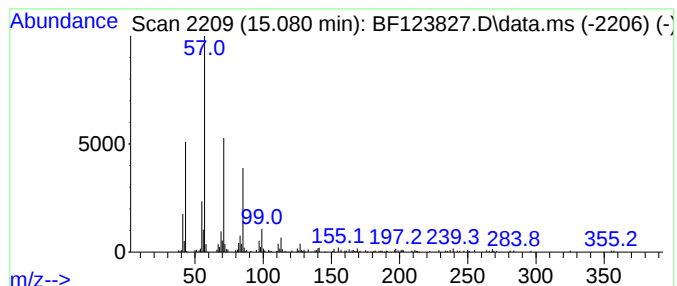
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	3.83 ng	250687	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Nonadecane	268	C19H40	000629-92-5	87
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	72
5			Heneicosane	296	C21H44	000629-94-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123827.D
Acq On : 5 May 2021 14:56
Operator : JU/CG
Sample : M2275-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CRT-020

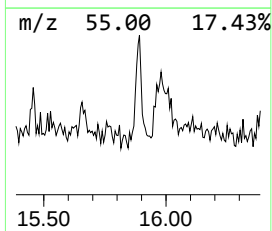
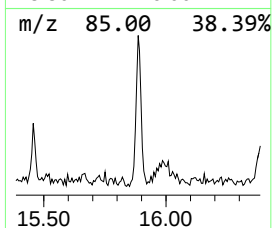
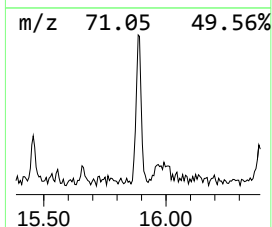
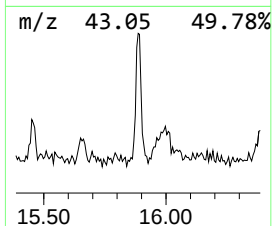
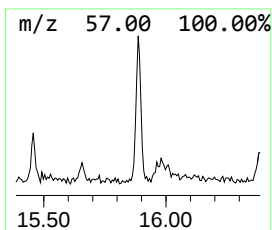
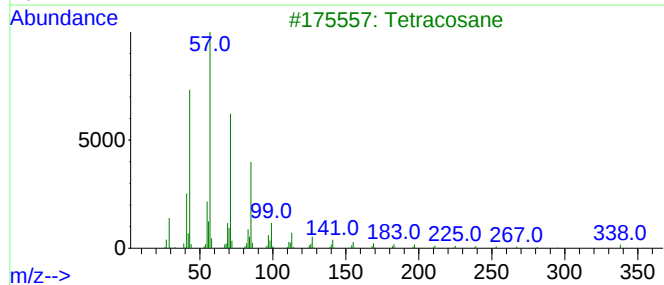
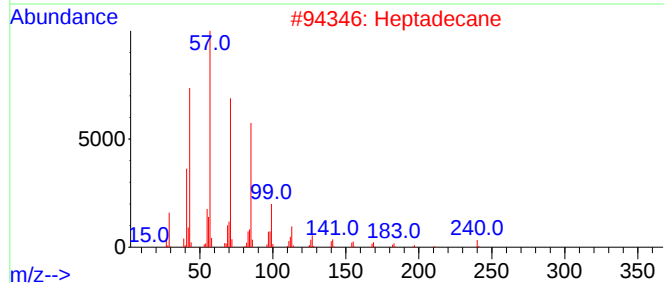
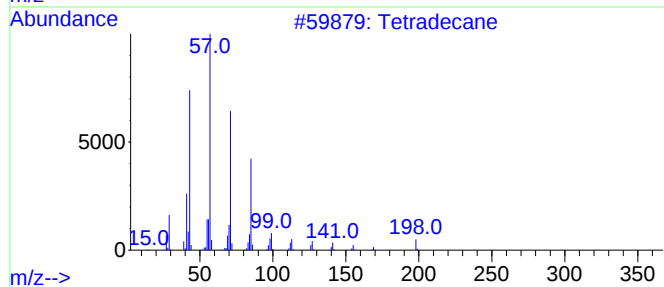
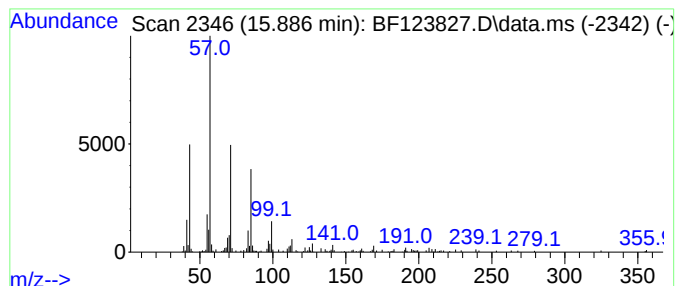
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	5.02 ng	328902	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	80
2			Heptadecane	240	C17H36	000629-78-7	80
3			Tetracosane	338	C24H50	000646-31-1	78
4			Hexadecane	226	C16H34	000544-76-3	78
5			Nonadecane	268	C19H40	000629-92-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123827.D
Acq On : 5 May 2021 14:56
Operator : JU/CG
Sample : M2275-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CRT-020

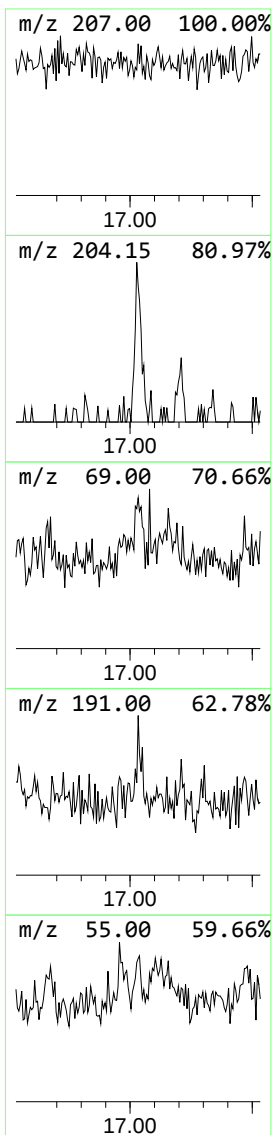
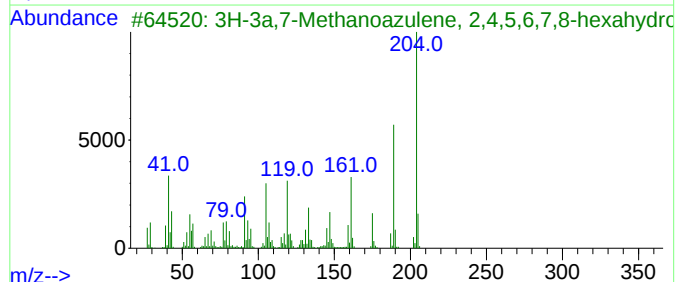
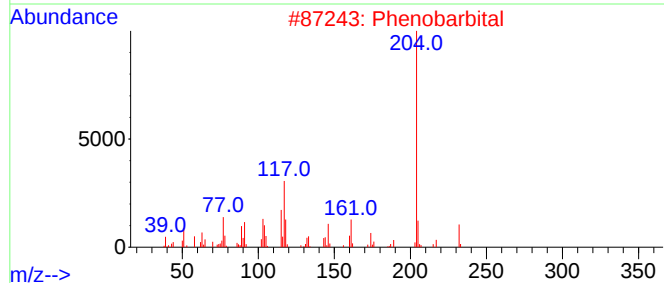
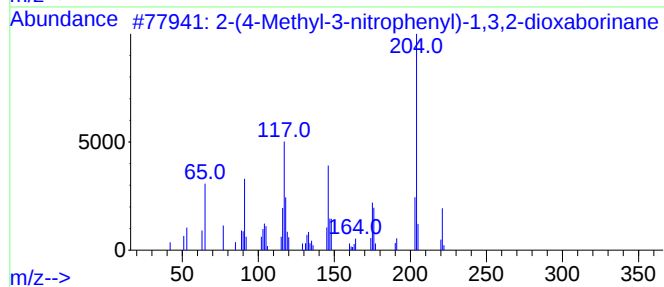
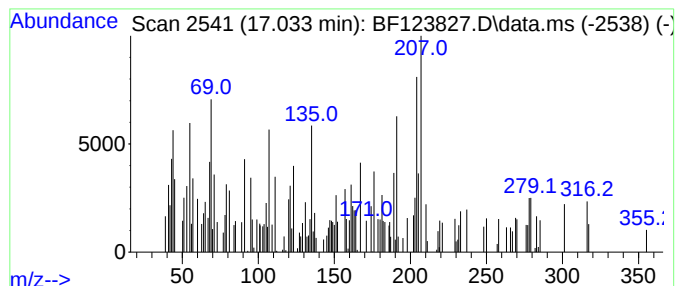
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown17.03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.033	2.02 ng	132243	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Methyl-3-nitrophenyl)-1,3,2...	221	C10H12BNO4	080279-22-7	44		
2	Phenobarbital	232	C12H12N2O3	000050-06-6	25		
3	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	15		
4	6-Nitro-8-methoxy-2H-chromene	207	C10H9NO4	062063-07-4	11		
5	3'-Carboxybenzo[1',2',-b]-1,4-di...	204	C11H12N2O2	138023-41-3	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123827.D
Acq On : 5 May 2021 14:56
Operator : JU/CG
Sample : M2275-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CRT-020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octane, 3,5-dim...	10.757	4.5	ng	443330	4	11.322	1980230	20.0
Dodecane, 2-met...	11.227	2.8	ng	271868	4	11.322	1980230	20.0
n-Hexadecanoic ...	11.857	3.3	ng	322074	4	11.322	1980230	20.0
Heptafluorobuty...	13.827	12.3	ng	898522	5	13.968	1460890	20.0
Cyclotetradecane	14.468	2.3	ng	166686	5	13.968	1460890	20.0
Heptacosane	15.080	3.8	ng	250687	6	15.421	1310220	20.0
Tetradecane	15.886	5.0	ng	328902	6	15.421	1310220	20.0
unknown17.03	17.033	2.0	ng	132243	6	15.421	1310220	20.0