LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139381.D
Acq On : 16 Sep 2024 16:30
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11930

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	12	21	30	rVB	912152	1446191	72.28%	9.064%
2	5.104	503	512	525	rBV	77529	121118	6.05%	0.759%
3	5.498	573	579	584	rBV	1273496	1727776	86.36%	10.829%
4	6.504	743	750	755	rBV	1254176	1810081	90.47%	11.345%
5	6.875	808	813	818	rBV	313132	372708	18.63%	2.336%
6	7.440	902	909	914	rBV	851522	1156112	57.79%	7.246%
7	7.687	947	951	956	rBB	31273	37963	1.90%	0.238%
8	8.157	1025	1031	1036	rBV	373564	457944	22.89%	2.870%
9	9.234	1208	1214	1219	rBV	1597922	2000706	100.00%	12.539%
10	9.910	1324	1329	1334	rBV	406197	500179	25.00%	3.135%
11	10.622	1444	1450	1457	rBV	113717	137019	6.85%	0.859%
12	10.698	1457	1463	1474	rBV	1003342	1282702	64.11%	8.039%
13	11.392	1576	1581	1589	rBV	426373	574428	28.71%	3.600%
14	11.463	1589	1593	1597	rBV	40101	51486	2.57%	0.323%
15	11.922	1662	1671	1676	rBV	278563	389995	19.49%	2.444%
16	12.004	1682	1685	1693	rVB	36236	61520	3.07%	0.386%
17	12.604	1782	1787	1793	rBV	315663	399306	19.96%	2.503%
18	12.698	1800	1803	1810	rBV	34944	53428	2.67%	0.335%
19	12.827	1818	1825	1830	rBV2	162302	273774	13.68%	1.716%
20	12.874	1830	1833	1839	rVB3	16868	25831	1.29%	0.162%
21	12.980	1841	1851	1856	rBV	1333054	1734289	86.68%	10.870%
22	13.051	1857	1863	1870	rBV5	17496	33525	1.68%	0.210%
23	13.157	1873	1881	1886	rVB	40723	68474	3.42%	0.429%
24	13.227	1886	1893	1896	rBV	35650	53674	2.68%	0.336%
25	13.663	1961	1967	1975	rBV	13023	20646	1.03%	0.129%
26	13.774	1981	1986	1989	rBV2	20005	28159	1.41%	0.176%
27	13.810	1989	1992	1998	rVV3	12546	23839	1.19%	0.149%
28	13.874	1998	2003	2013	rVV4	38167	80237	4.01%	0.503%
29	14.027	2021	2029	2041	rVB3	276019	575174	28.75%	3.605%
30	14.880	2169	2174	2182	rVB	24703	35757	1.79%	0.224%
31	15.063	2200	2205	2214	rBV	37030	78123	3.90%	0.490%
32	15.368	2252	2257	2262	rVB	16784	24648	1.23%	0.154%
33	15.427	2262	2267	2272	rVV	19503	29388	1.47%	0.184%
34	15.492	2272	2278	2294	rVB	181410	289198	14.45%	1.813%

Sum of corrected areas: 15955398

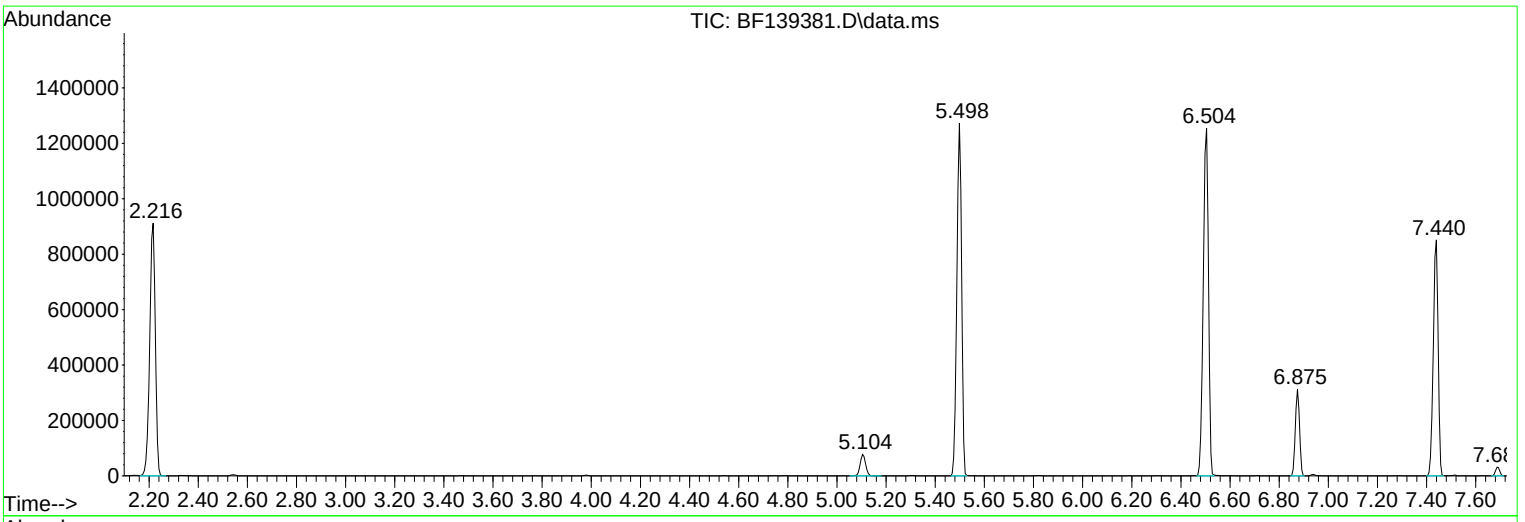
Instrument :
BNA_F
ClientSampleId :
72-11930

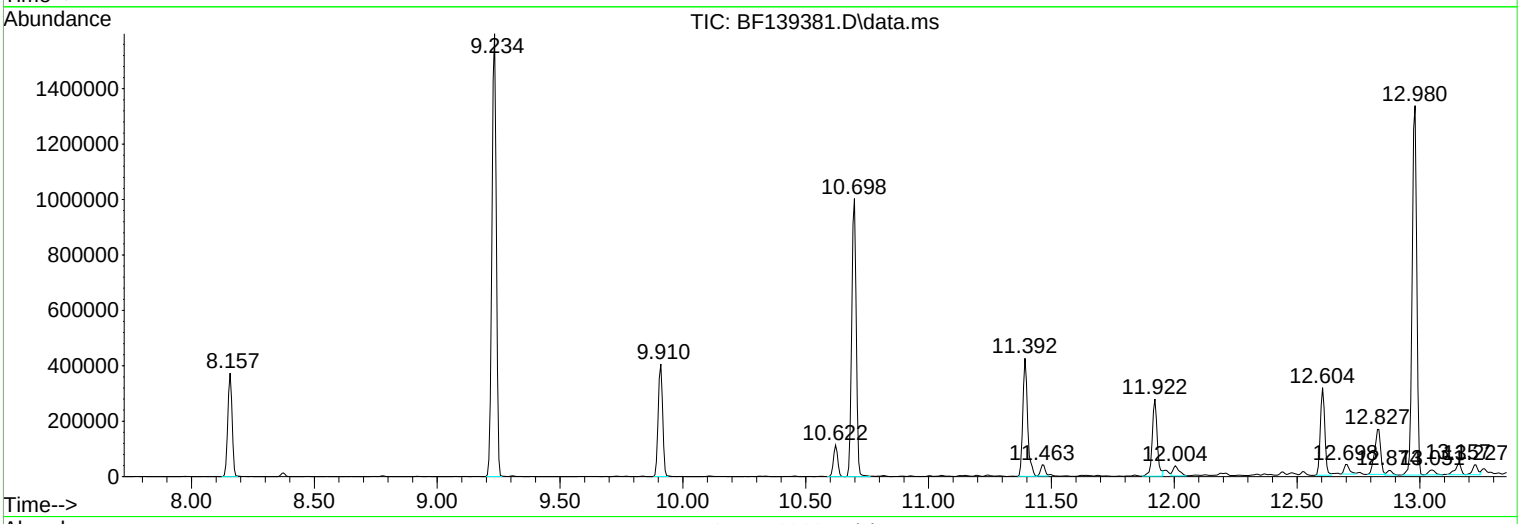
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091624\
Data File : BF139381.D
Acq On : 16 Sep 2024 16:30
Operator : RC/JU
Sample : P3929-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

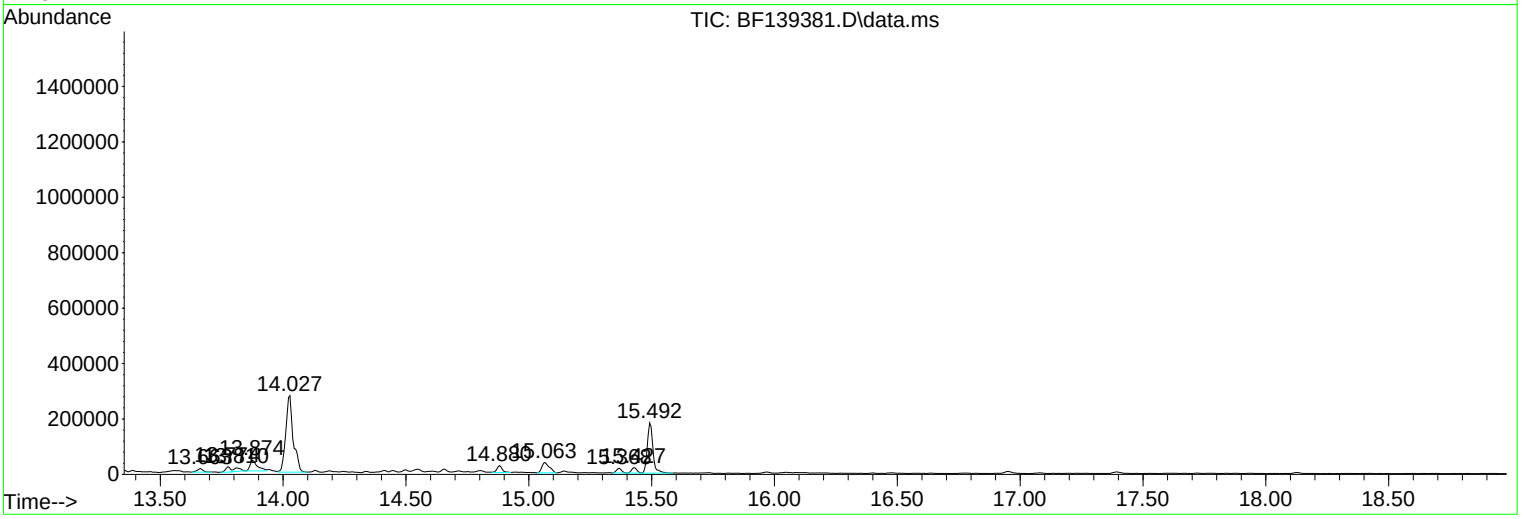
Instrument :
BNA_F
ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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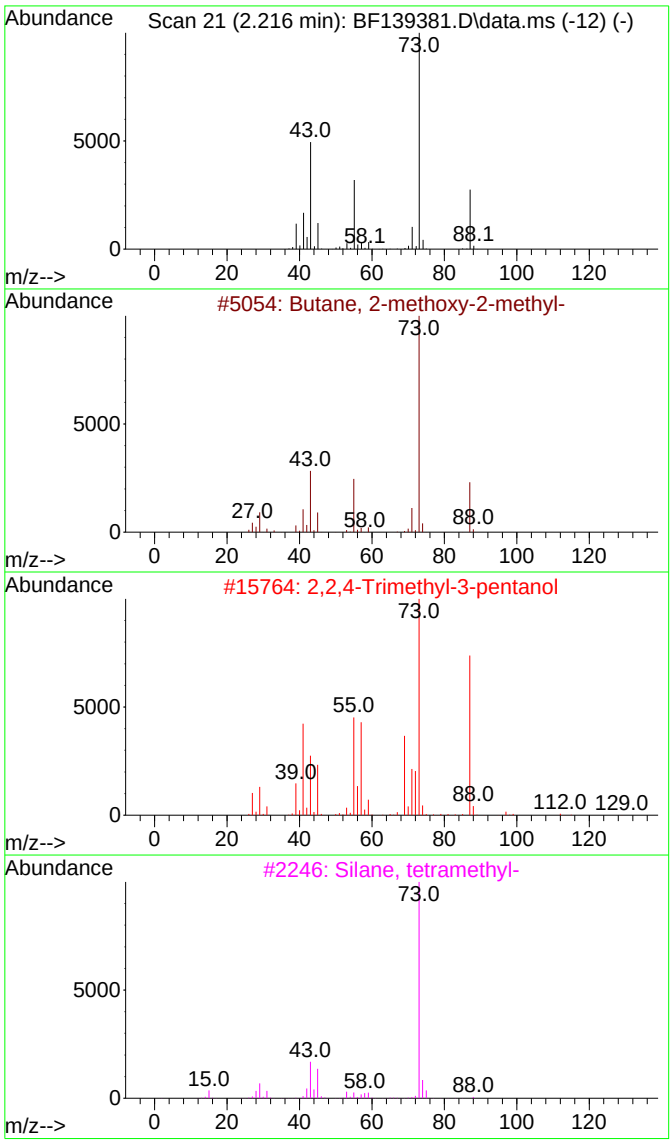
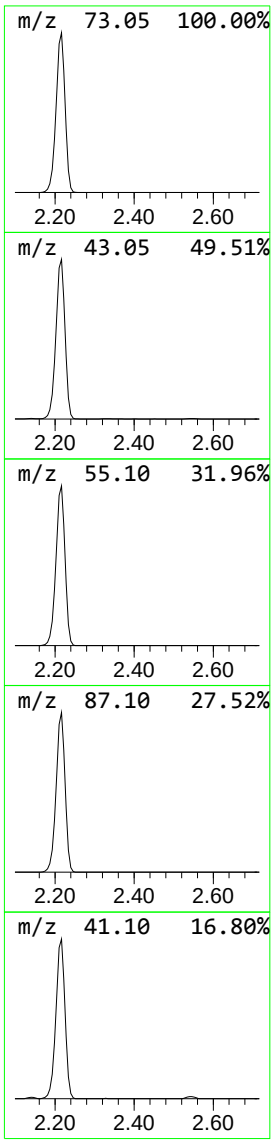
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	77.60 ng	1446190	1,4-Dichlorobenzene-d4	6.875

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	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BF139381.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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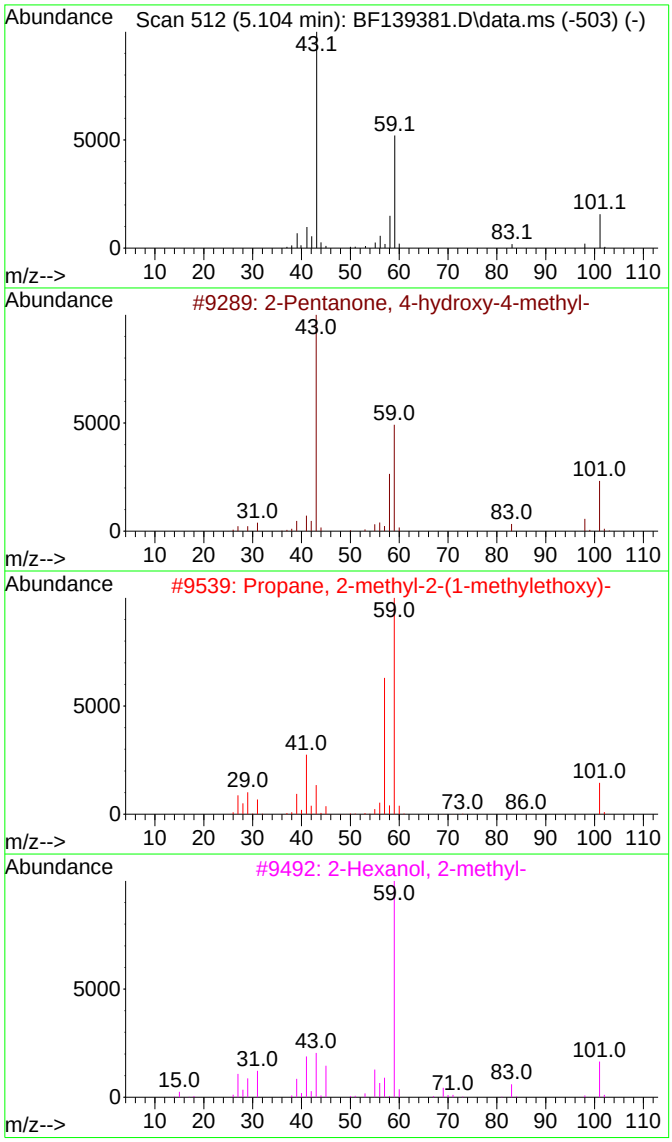
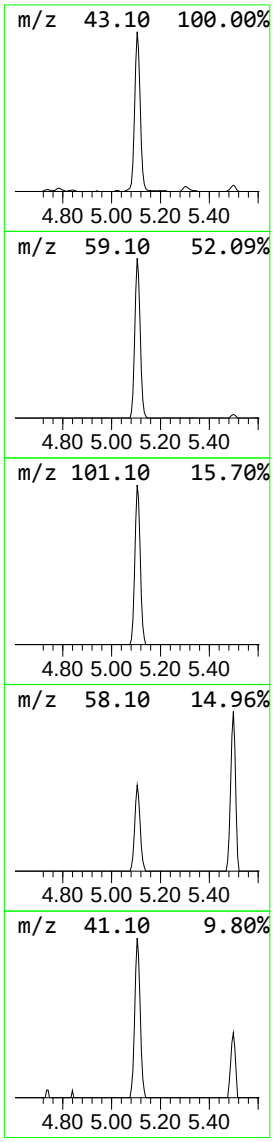
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	6.50 ng	121118	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

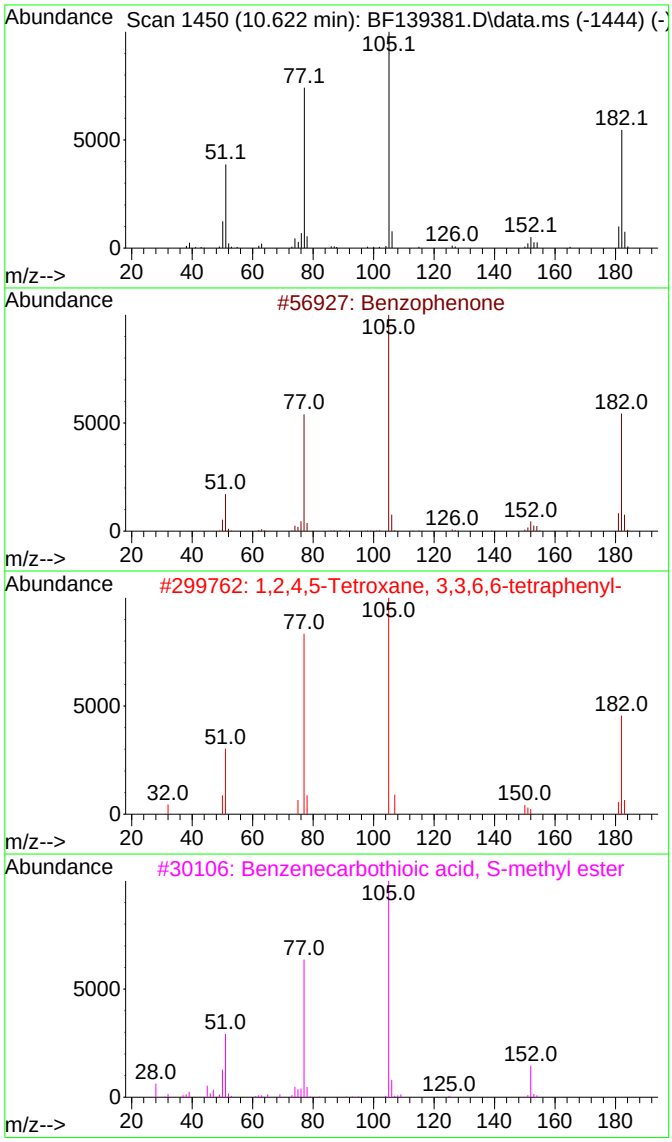
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

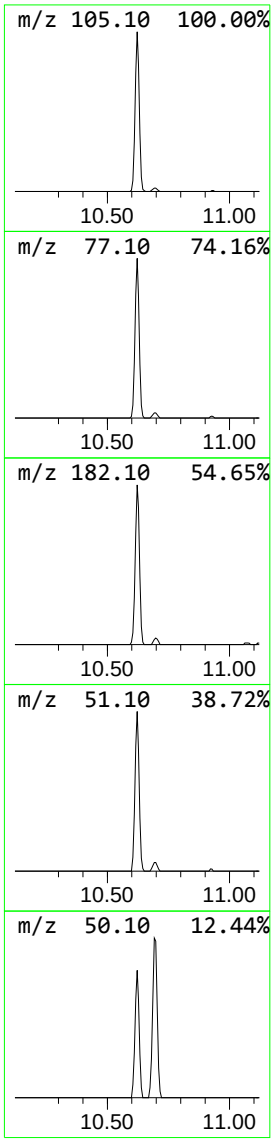
****

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.48 ng	137019	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	83
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
4	Benzoylformic acid	150	C8H6O3	000611-73-4	58
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	53





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Instrument :
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ClientSampleId :
72-11930

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
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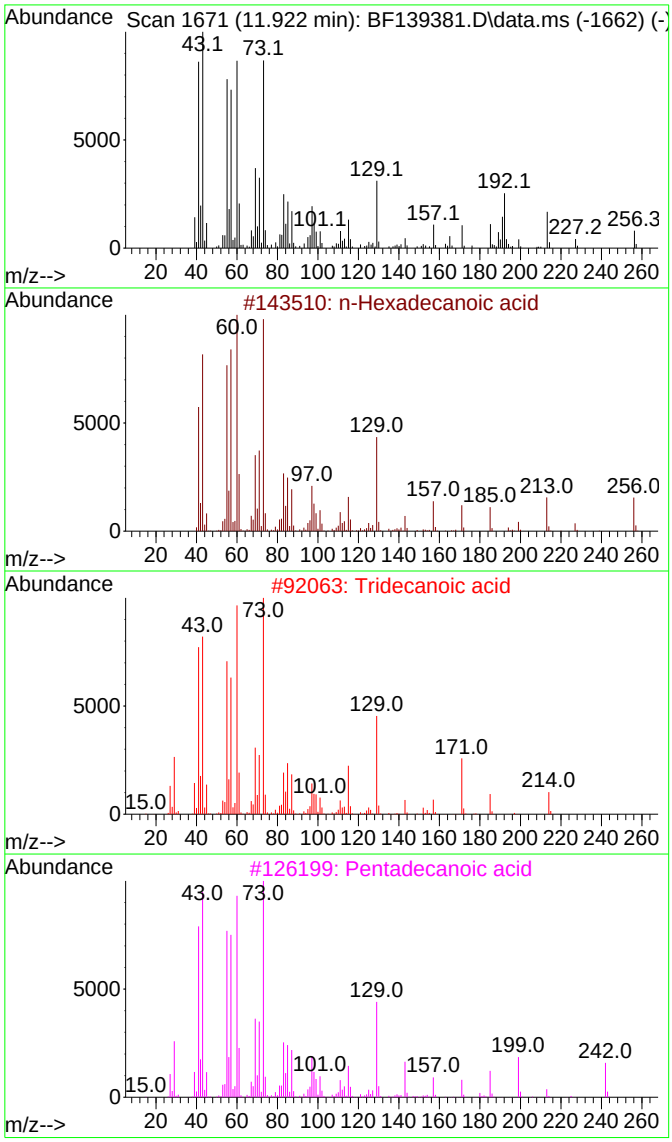
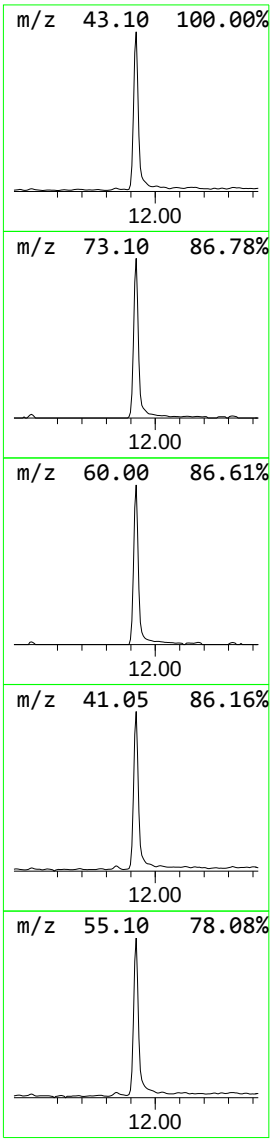
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	13.58 ng	389995	Phenanthrene-d10	11.392

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Instrument :
BNA_F
ClientSampleId :
72-11930

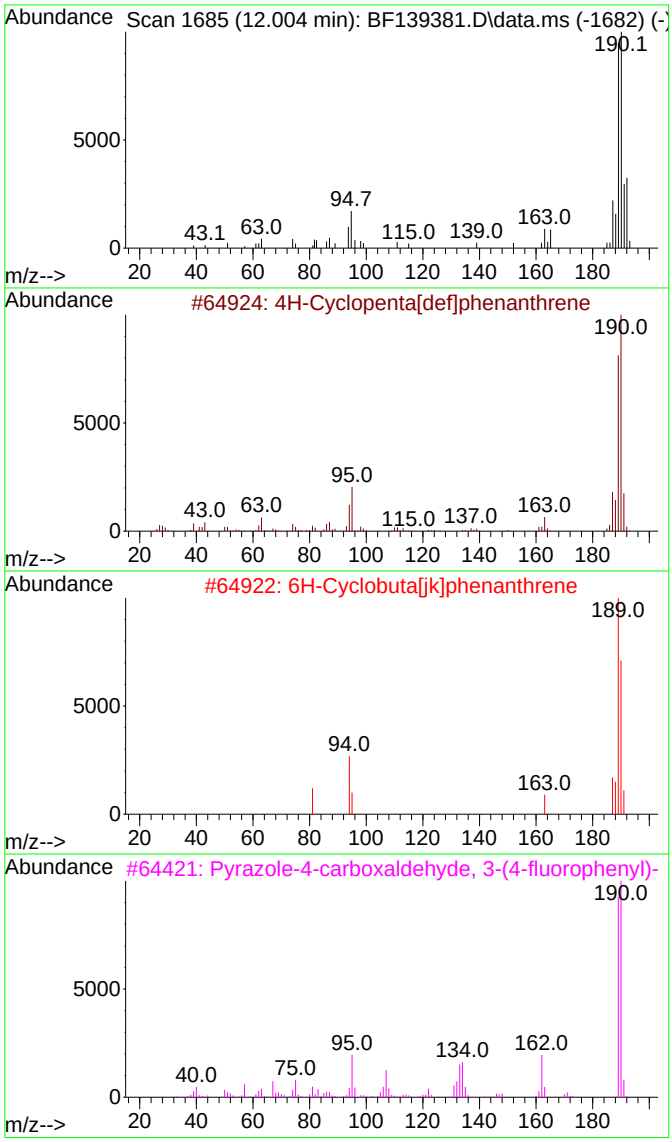
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

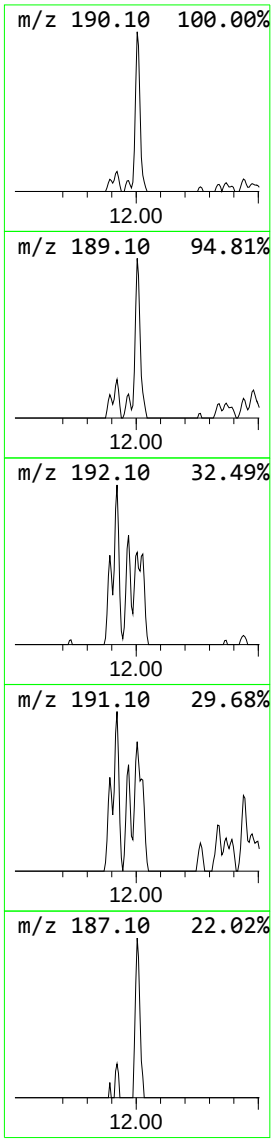
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.14 ng	61520	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
4	Pyrimidine, 6-oxo-4-(4-fluorophe...	190	C10H7FN2O	085979-57-3	17
5	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	9





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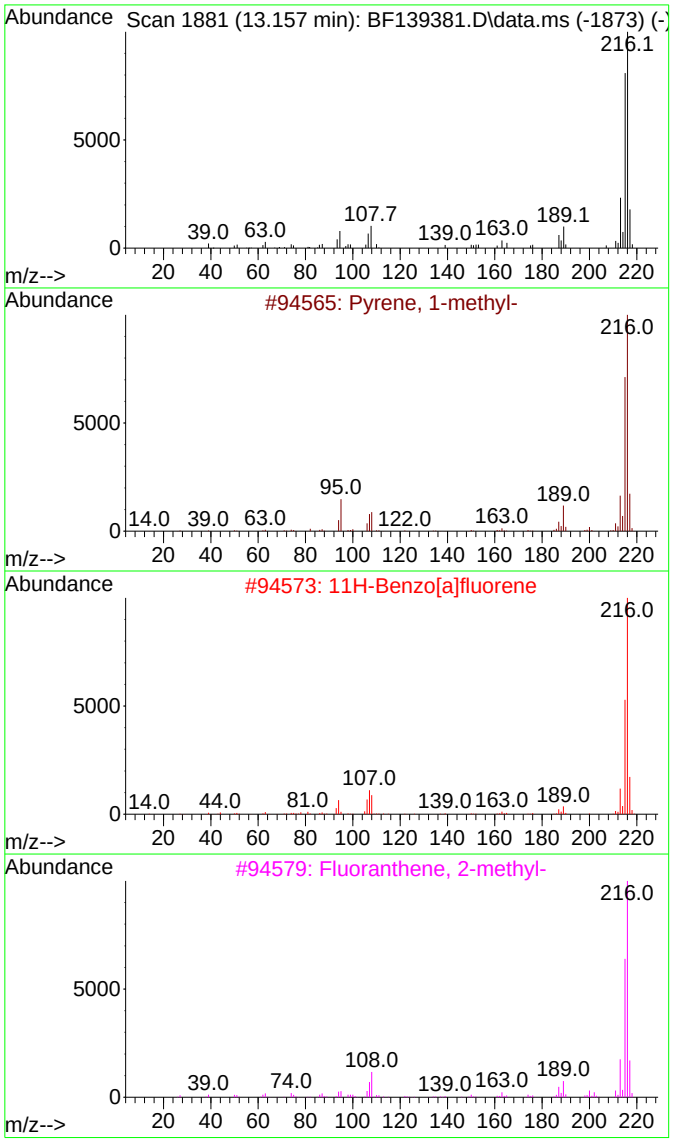
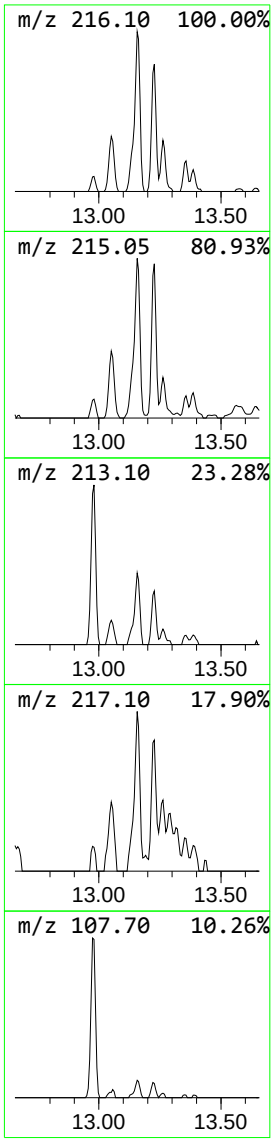
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	2.38 ng	68474	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	97
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





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Operator : RC/JU
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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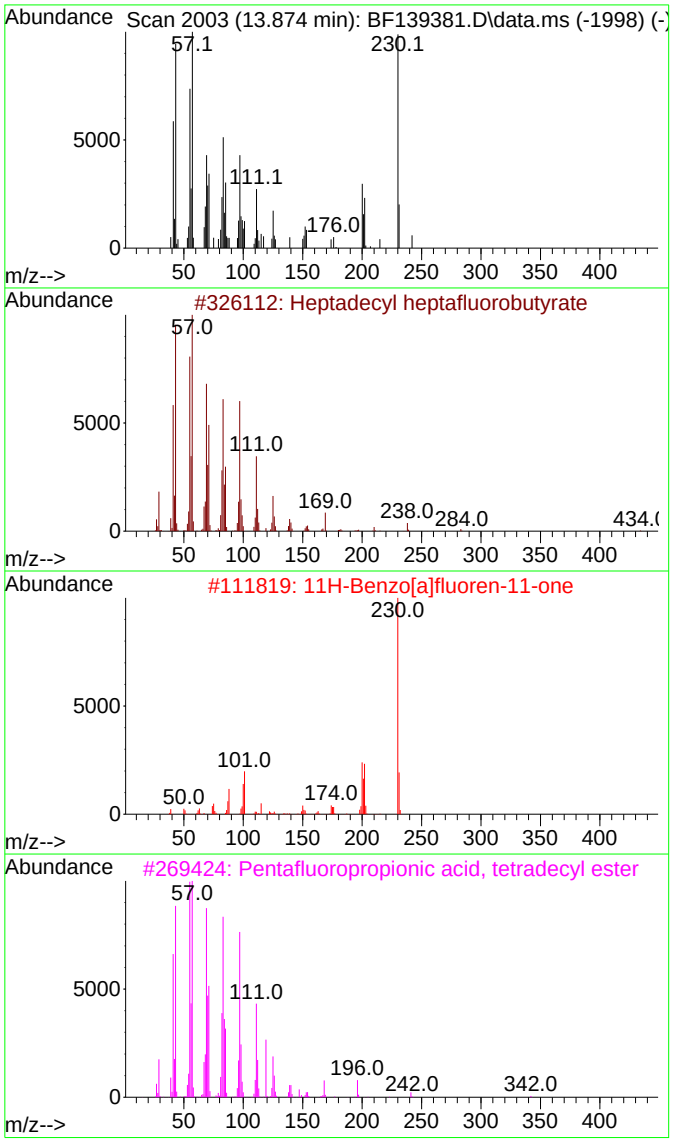
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

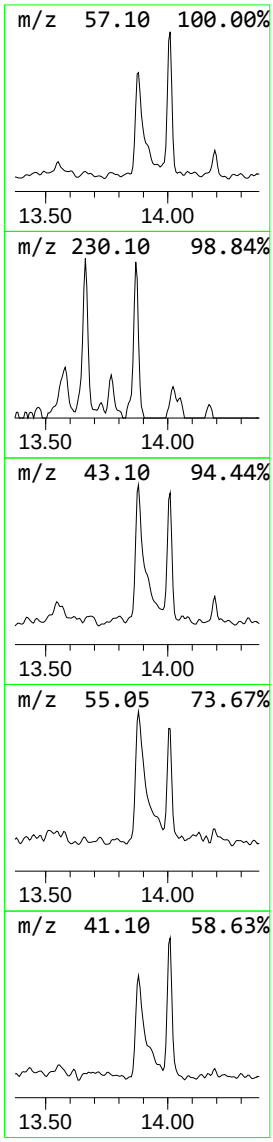
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.79 ng	80237	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	80
2	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	50
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	42
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	42
5	1-Heneicosanol	312	C21H44O	015594-90-8	42





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

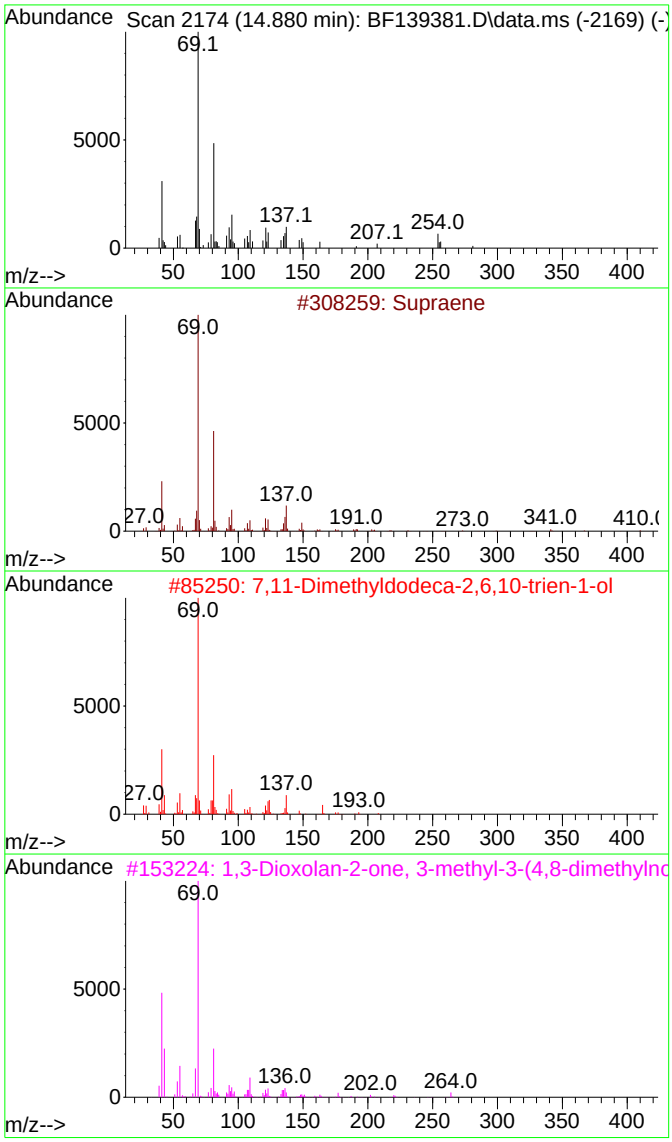
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

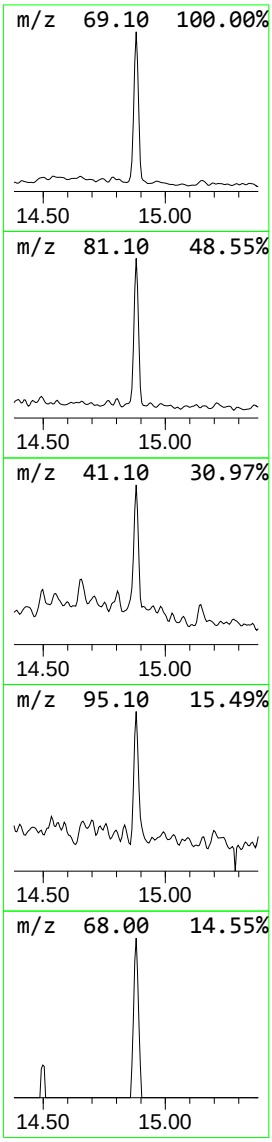
****

Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.47 ng	35757	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	72
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3	1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	59
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
5	2H-1-Benzopyran-2-one, 7-[(3,7-d...	298	C19H22O3	000495-02-3	59





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.216	77.6	ng	1446190	1	6.875	372708	20.0
2-Pentanone, 4-...	5.104	6.5	ng	121118	1	6.875	372708	20.0
Benzophenone	10.622	5.5	ng	137019	3	9.910	500179	20.0
n-Hexadecanoic ...	11.922	13.6	ng	389995	4	11.392	574428	20.0
4H-Cyclopenta[d...	12.004	2.1	ng	61520	4	11.392	574428	20.0
Pyrene, 1-methyl-	13.157	2.4	ng	68474	5	14.027	575174	20.0
Heptadecyl hept...	13.874	2.8	ng	80237	5	14.027	575174	20.0
Supraene	14.880	2.5	ng	35757	6	15.492	289198	20.0