LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(6-10)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124214.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	17	20	24	rBB2	12616	13696	1.73%	0.191%
2	5.057	502	505	512	rVB2	48942	54683	6.90%	0.761%
3	5.481	573	577	587	rBB	584924	534697	67.49%	7.446%
4	6.492	745	749	758	rVB	618589	560695	70.77%	7.808%
5	6.851	806	810	813	rBB	252426	217513	27.45%	3.029%
6	7.410	901	905	908	rBV	494748	389978	49.22%	5.431%
7	8.133	1024	1028	1030	rBV	317878	278547	35.16%	3.879%
8	9.204	1206	1210	1214	rBV	893991	792274	100.00%	11.033%
9	9.598	1274	1277	1280	rBV	143493	105252	13.28%	1.466%
10	9.745	1295	1302	1306	rBB	13420	11649	1.47%	0.162%
11	9.886	1322	1326	1329	rVB	443274	333719	42.12%	4.647%
12	10.092	1358	1361	1365	rVB2	14069	12218	1.54%	0.170%
13	10.433	1416	1419	1425	rVB2	14043	15185	1.92%	0.211%
14	10.674	1457	1460	1464	rBV	471129	408575	51.57%	5.690%
15	10.786	1475	1479	1480	rBV	11169	9343	1.18%	0.130%
16	11.180	1543	1546	1550	rVB	18038	16337	2.06%	0.228%
17	11.233	1550	1555	1558	rBV4	13743	17682	2.23%	0.246%
18	11.268	1558	1561	1564	rVV2	17227	14953	1.89%	0.208%
19	11.374	1575	1579	1581	rBV	370988	311198	39.28%	4.334%
20	11.398	1581	1583	1586	rVV	255945	189726	23.95%	2.642%
21	11.445	1588	1591	1595	rVB	34289	33116	4.18%	0.461%
22	11.610	1612	1619	1621	rBV4	13869	17967	2.27%	0.250%
23	11.663	1625	1628	1633	rVB2	24888	23258	2.94%	0.324%
24	11.710	1633	1636	1640	rBV4	7177	10006	1.26%	0.139%
25	11.833	1652	1657	1659	rBV4	5807	8730	1.10%	0.122%
26	11.874	1661	1664	1666	rBV3	25975	24029	3.03%	0.335%
27	11.904	1666	1669	1672	rVV	43091	39663	5.01%	0.552%
28	11.951	1675	1677	1680	rVV4	11678	15020	1.90%	0.209%
29	11.986	1680	1683	1686	rVV4	26897	33832	4.27%	0.471%
30	12.010	1686	1687	1691	rVB4	17564	12531	1.58%	0.174%
31	12.068	1695	1697	1704	rBV	27774	28762	3.63%	0.401%
32	12.168	1711	1714	1717	rBV2	18561	16869	2.13%	0.235%
33	12.198	1717	1719	1721	rVB3	17382	13458	1.70%	0.187%
34	12.315	1736	1739	1742	rBV4	9247	12145	1.53%	0.169%
35	12.421	1755	1757	1760	rBV3	14384	15056	1.90%	0.210%
36	12.457	1760	1763	1766	rVV3	32555	30967	3.91%	0.431%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(6-10)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.510	1770	1772	1777	rVB4	22243	22207	2.80%	0.309%
38	12.586	1782	1785	1790	rVB	242979	206649	26.08%	2.878%
39	12.686	1799	1802	1803	rBV	18812	14251	1.80%	0.198%
40	12.815	1819	1824	1831	rBV	186209	218600	27.59%	3.044%
41	12.862	1831	1832	1836	rVB4	13589	13277	1.68%	0.185%
42	12.957	1842	1848	1851	rBV	784407	671484	84.75%	9.351%
43	13.039	1858	1862	1865	rVB6	12743	18909	2.39%	0.263%
44	13.121	1874	1876	1878	rBV3	19821	17995	2.27%	0.251%
45	13.145	1878	1880	1883	rVB4	24700	21451	2.71%	0.299%
46	13.186	1883	1887	1890	rBV4	35055	45336	5.72%	0.631%
47	13.251	1895	1898	1903	rVV6	25887	33110	4.18%	0.461%
48	13.339	1911	1913	1916	rBV4	14313	16451	2.08%	0.229%
49	13.368	1916	1918	1921	rBV4	9886	11230	1.42%	0.156%
50	13.439	1926	1930	1933	rBV	70227	79517	10.04%	1.107%
51	13.527	1943	1945	1951	rVB6	30768	34066	4.30%	0.474%
52	13.627	1960	1962	1964	rBV3	15042	17405	2.20%	0.242%
53	13.657	1964	1967	1968	rVB3	23752	22899	2.89%	0.319%
54	13.762	1983	1985	1989	rBV4	20644	19699	2.49%	0.274%
55	13.857	1999	2001	2013	rBV10	45002	119549	15.09%	1.665%
56	14.015	2024	2028	2031	rBV2	302293	343039	43.30%	4.777%
57	14.045	2031	2033	2038	rVB	88399	76773	9.69%	1.069%
58	14.762	2153	2155	2159	rBV3	46179	51257	6.47%	0.714%
59	15.062	2202	2206	2213	rVB2	72393	133019	16.79%	1.852%
60	15.433	2266	2269	2275	rVB	53184	68938	8.70%	0.960%
61	15.492	2275	2279	2288	rBV	157922	271397	34.26%	3.779%
62	18.933	2862	2864	2867	rVB4	13881	9254	1.17%	0.129%

Sum of corrected areas: 7181091

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
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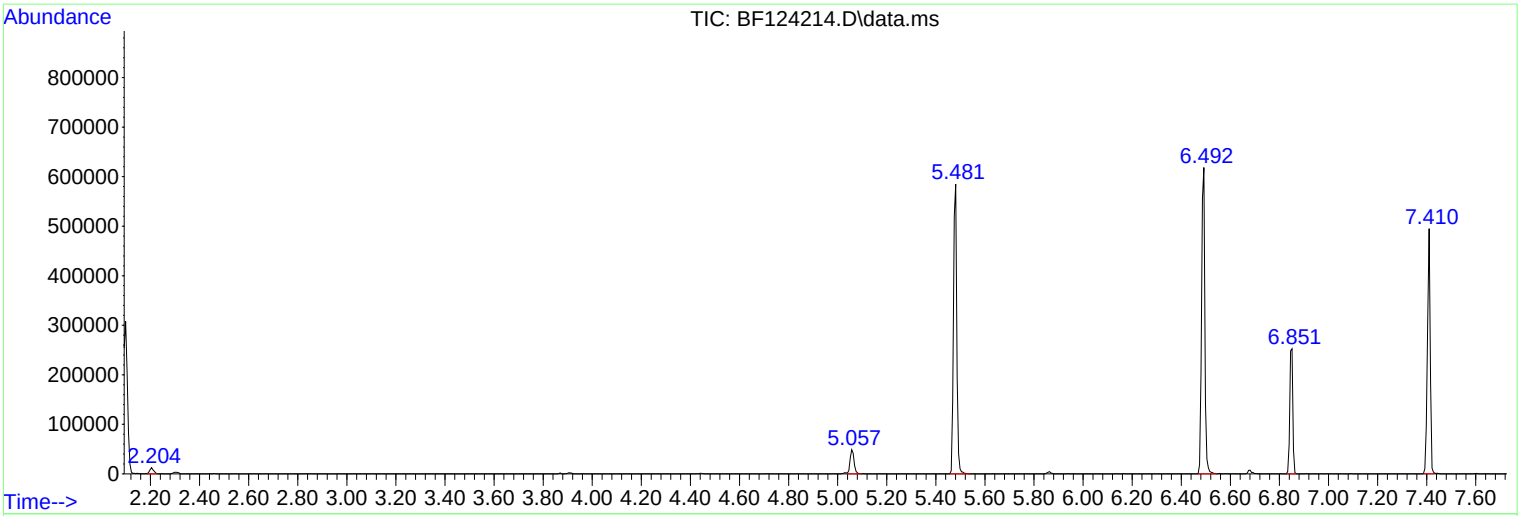
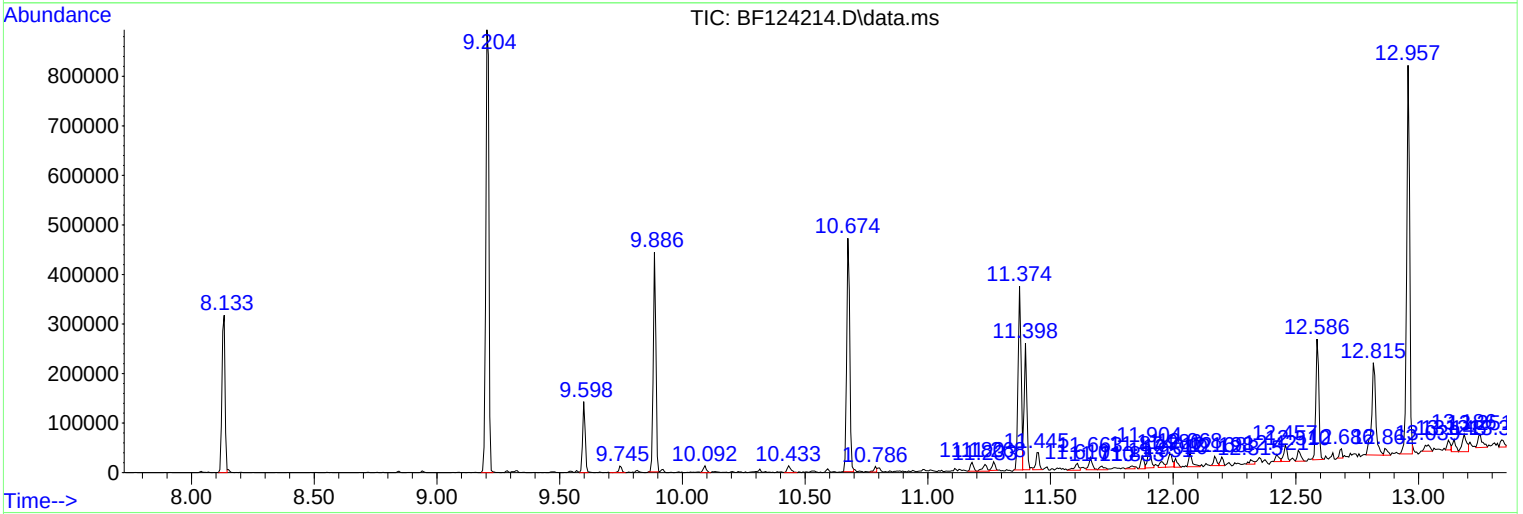
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

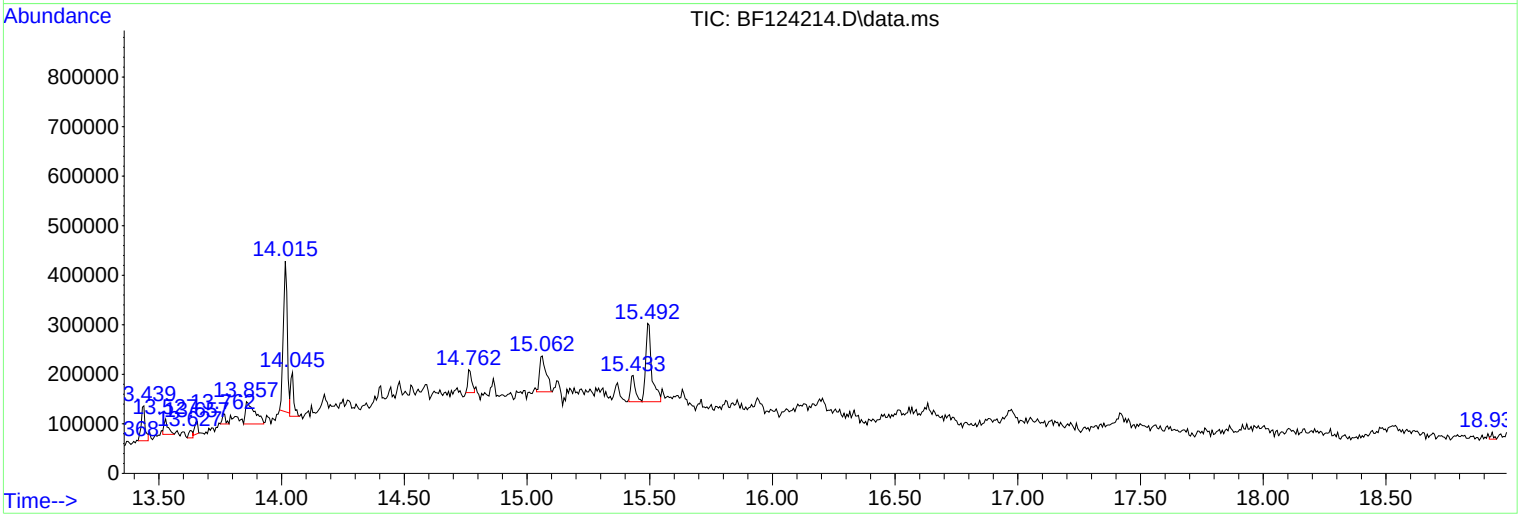
Instrument :
BNA_F
ClientSampleId :
18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
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BNA_F
ClientSampleId :
18-B12(6-10)

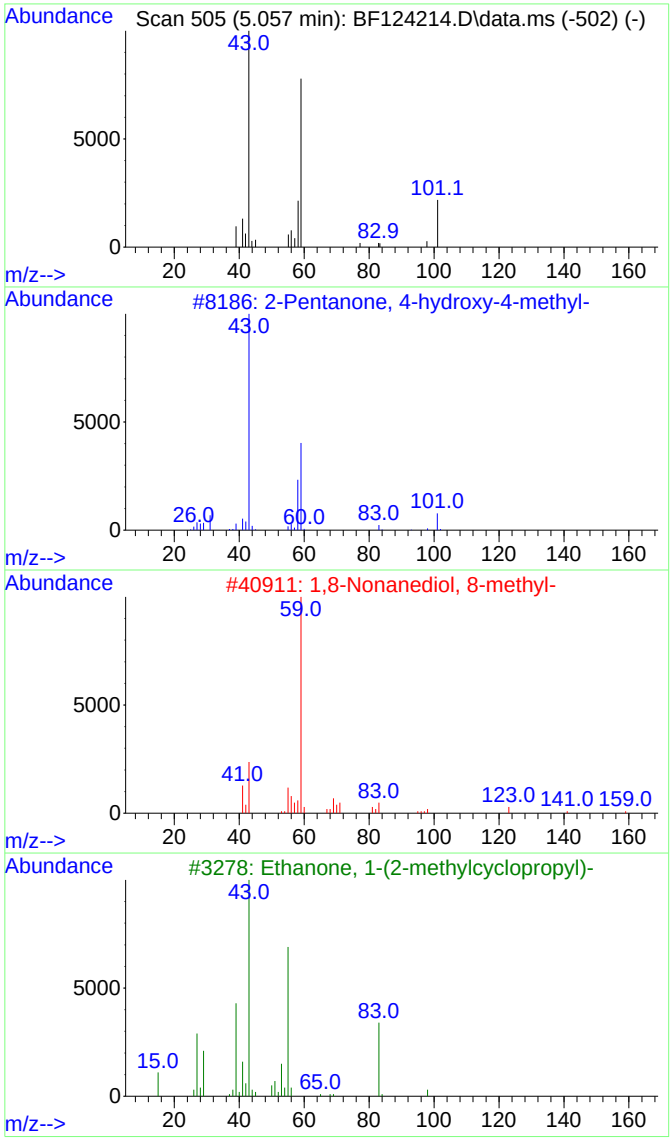
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

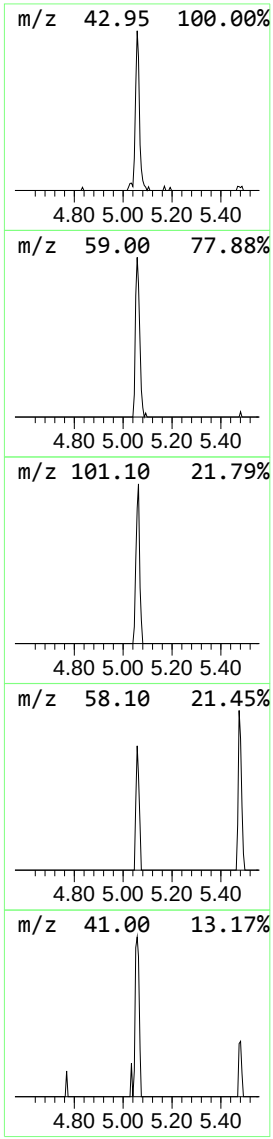
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	5.03 ng	54683	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

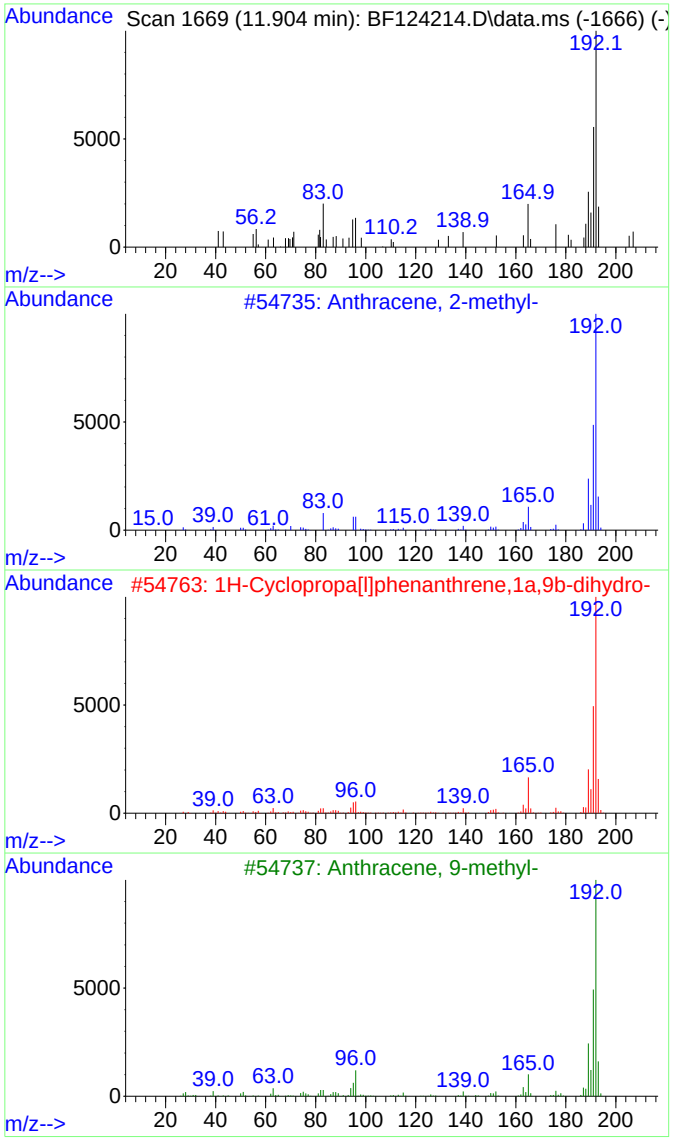
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

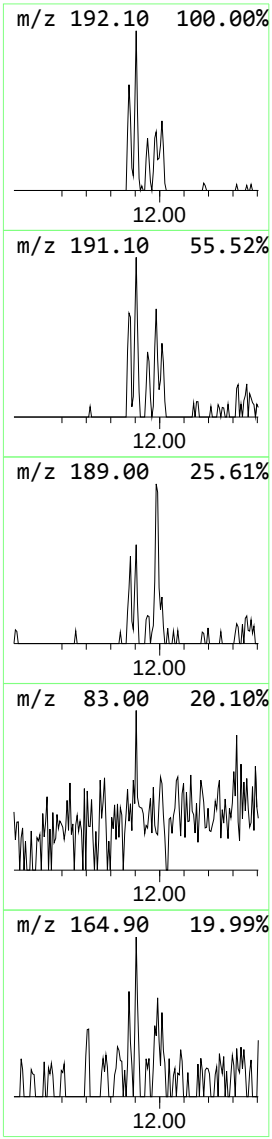
****

Peak Number 2 Anthracene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.55 ng	39663	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	87
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	87
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(6-10)

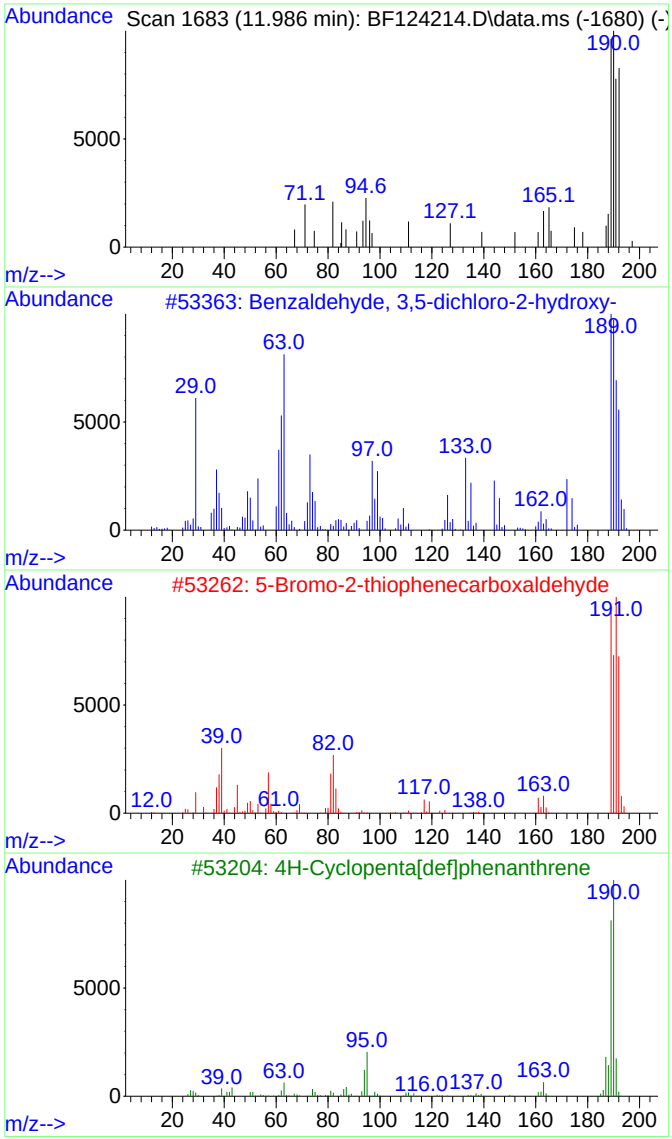
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

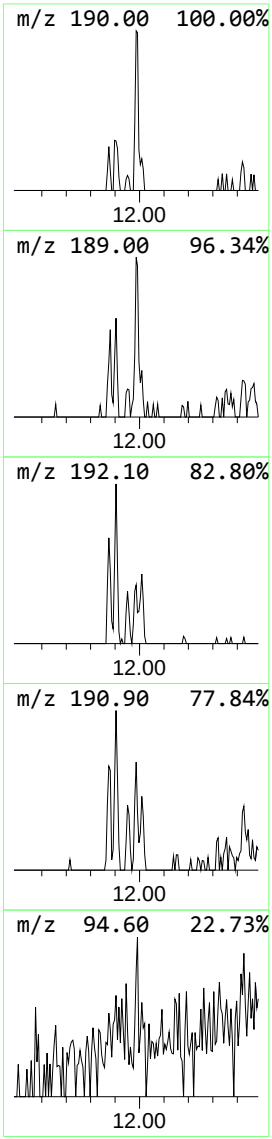
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzaldehyde, 3,5-dichloro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.17 ng	33832	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
2	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	53
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	38
4	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	38
5	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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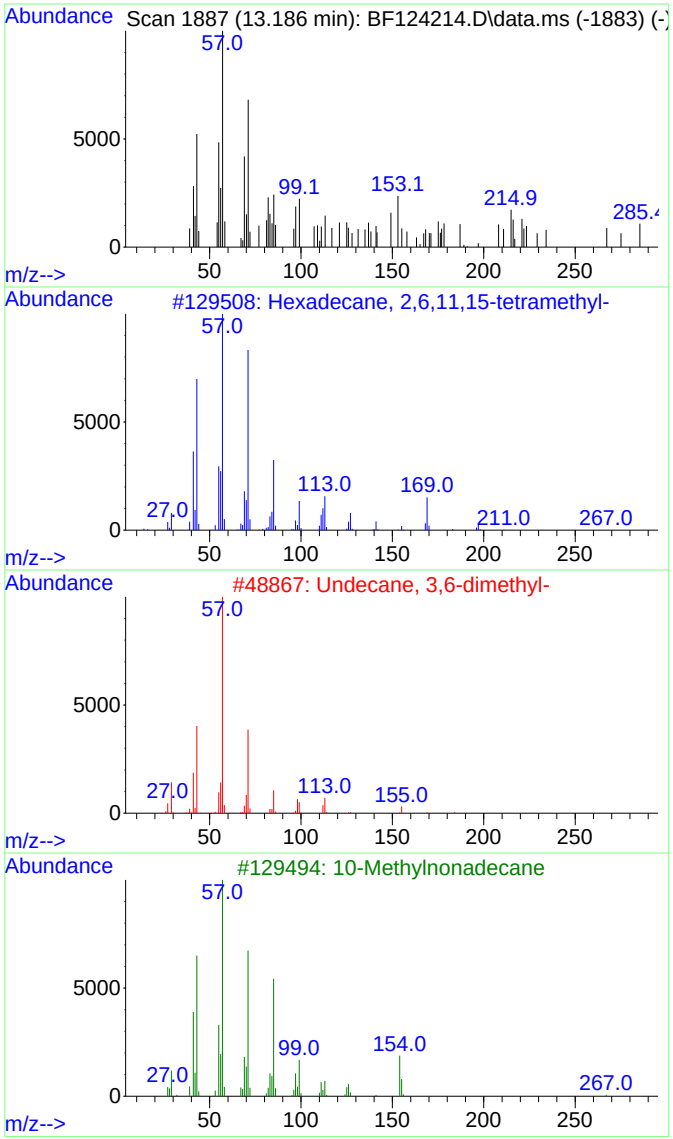
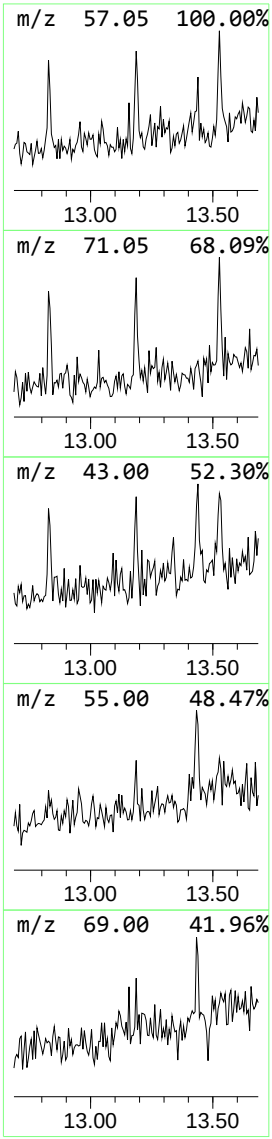
****

Peak Number 4 unknown13.186 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.186	2.64 ng	45336	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	35
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	35
3	10-Methylnonadecane	282	C20H42	056862-62-5	30
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	27
5	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

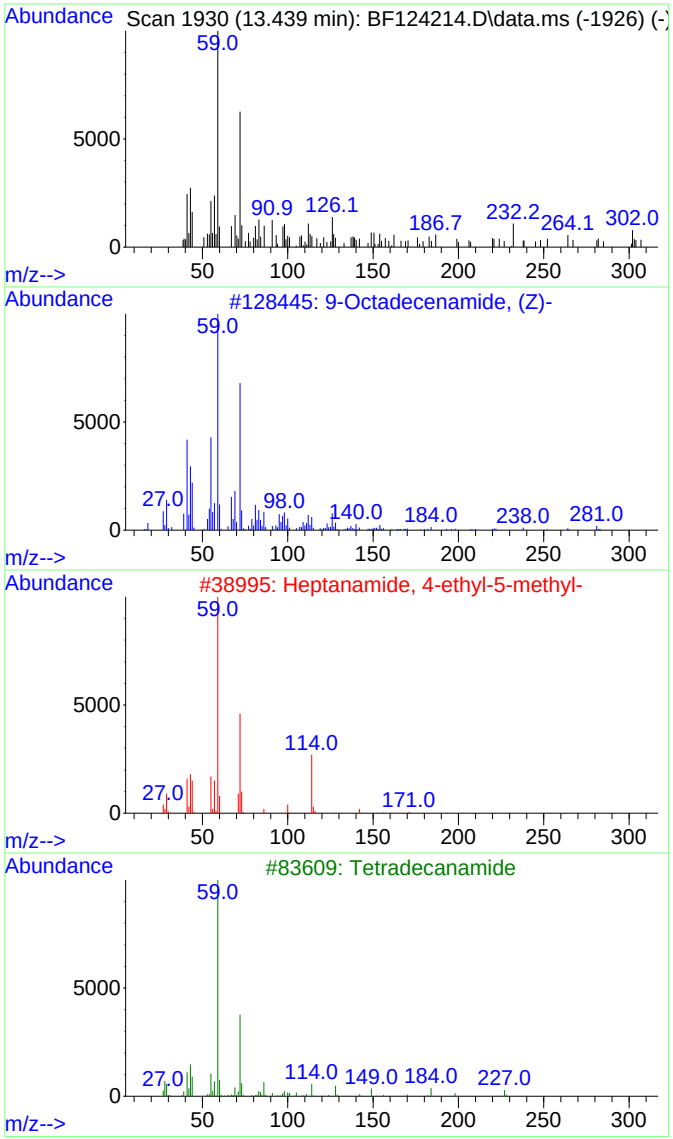
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

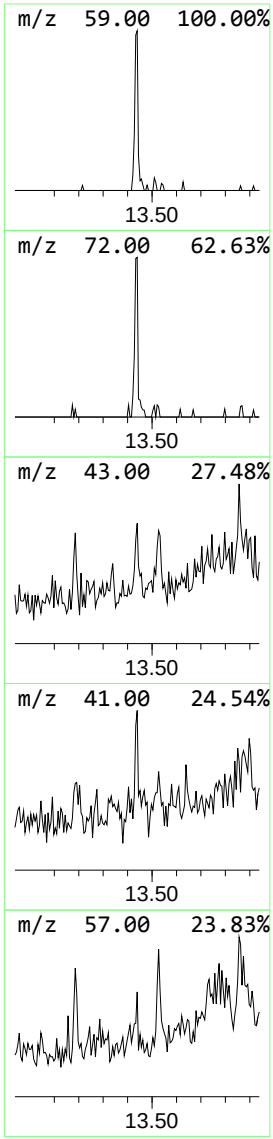
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.439	4.64 ng	79517	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	92
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
3	Tetradecanamide	227	C14H29NO	000638-58-4	49
4	Octanamide	143	C8H17NO	000629-01-6	47
5	Hydrazine, 1,1-dimethyl-2-(1-met...	116	C6H16N2	054007-24-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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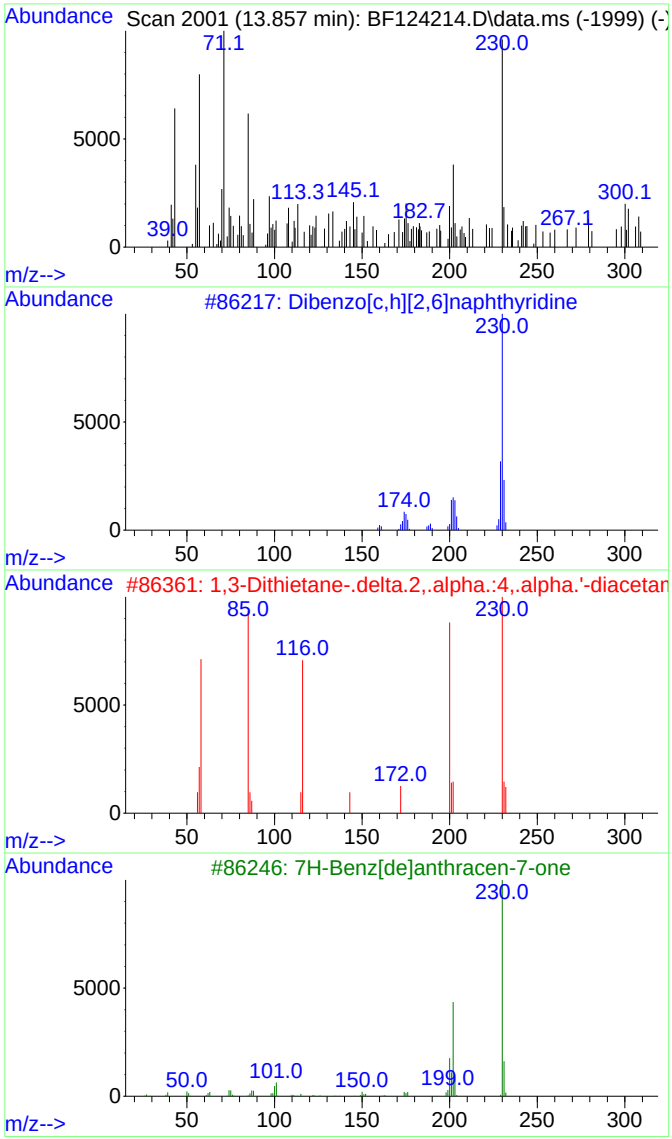
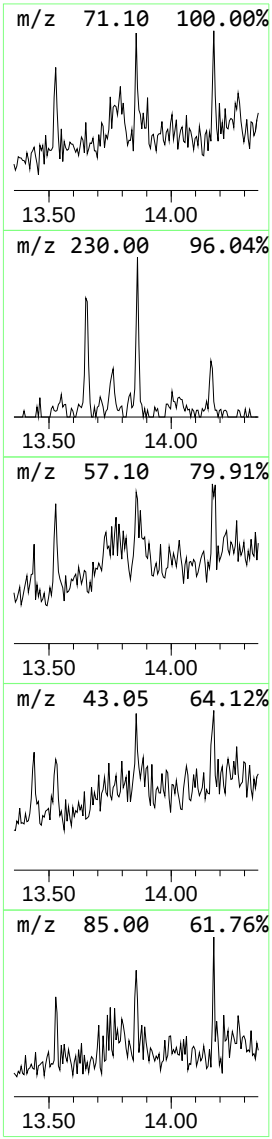
Peak Number 6 unknown13.857 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	6.97 ng	119549	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	35
2	1,3-Dithietane-.delta.2,.alpha.:...	230	C8H10N2O2S2	027123-79-1	30
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	30
4	Stilbene, 2-hydroxy-4'-chloro-, ...	230	C14H11ClO	1000138-48-2	27
5	2,2-Dimethyl-3,4-dihydro-2H,5H-p...	230	C14H14O3	031490-68-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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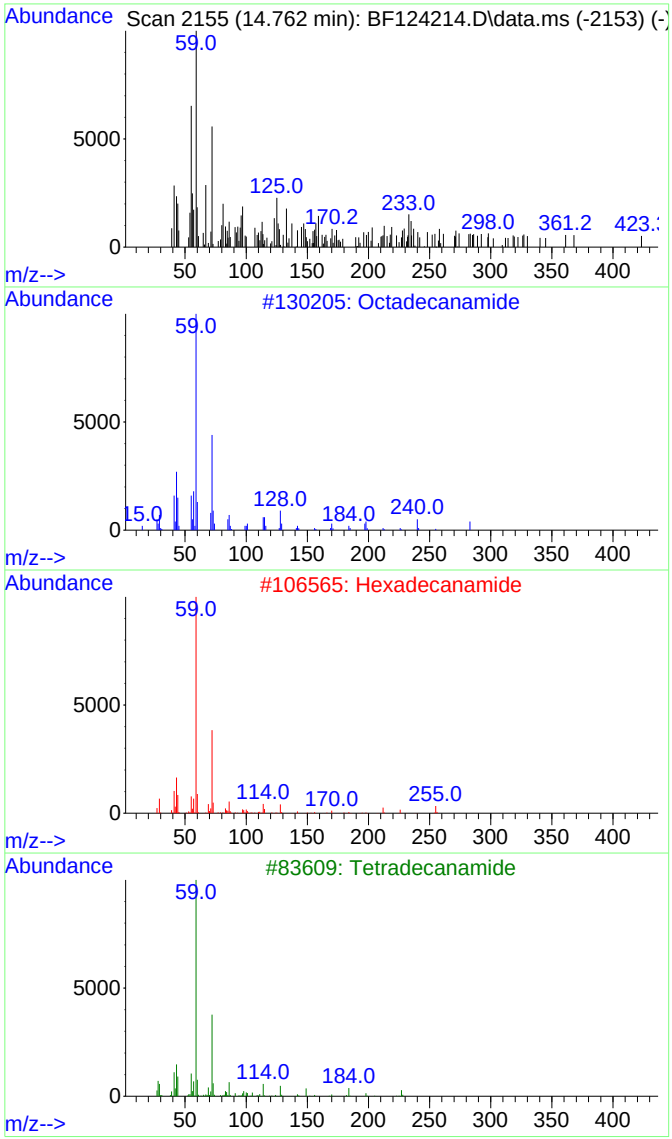
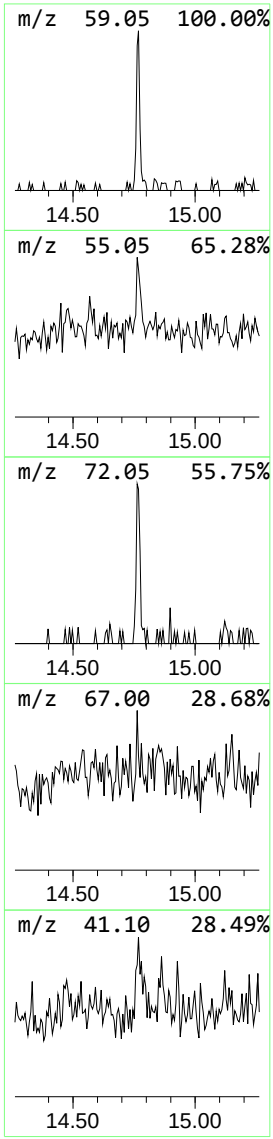
Peak Number 7 Octadecanamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	3.78 ng	51257	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanamide	283	C18H37NO	000124-26-5	60
2	Hexadecanamide	255	C16H33NO	000629-54-9	47
3	Tetradecanamide	227	C14H29NO	000638-58-4	47
4	Nonadecanamide	297	C19H39NO	058185-32-3	38
5	Succinic acid, 2-methylphenyl 2-...	266	C14H18O5	1000357-53-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124214.D
Acq On : 9 Jun 2021 18:06
Operator : JU/CG
Sample : M2612-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 18-B12(6-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	5.0	ng	54683	1	6.851	217513	20.0
Anthracene, 2-m...	11.904	2.5	ng	39663	4	11.374	311198	20.0
Benzaldehyde, 3...	11.986	2.2	ng	33832	4	11.374	311198	20.0
unknown13.186	13.186	2.6	ng	45336	5	14.015	343039	20.0
9-Octadecenamid...	13.439	4.6	ng	79517	5	14.015	343039	20.0
unknown13.857	13.857	7.0	ng	119549	5	14.015	343039	20.0
Octadecanamide	14.762	3.8	ng	51257	6	15.492	271397	20.0