LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129912.D
Acq On : 19 Aug 2022 15:12
Operator : CG\JU
Sample : N4225-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R-70-1

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.005	459	462	479	rVB	207721	268519	8.79%	1.333%
2	5.428	530	534	553	rBV	2744164	2787781	91.22%	13.840%
3	6.446	704	707	721	rBV	2698218	2755940	90.18%	13.682%
4	6.793	762	766	772	rBV	1004102	816202	26.71%	4.052%
5	7.363	858	863	866	rBV	2033815	1764441	57.73%	8.759%
6	8.075	980	984	988	rBV	1359120	1041382	34.08%	5.170%
7	9.152	1161	1167	1170	rBV	3812615	3056115	100.00%	15.172%
8	9.834	1279	1283	1286	rBV	1123811	1017544	33.30%	5.052%
9	10.628	1414	1418	1426	rBV	1708050	1436082	46.99%	7.129%
10	10.722	1431	1434	1444	rVB2	36985	63863	2.09%	0.317%
11	11.322	1533	1536	1539	rBV	1000254	805328	26.35%	3.998%
12	11.346	1539	1540	1544	rVB	52275	37509	1.23%	0.186%
13	11.840	1619	1624	1629	rBV3	40587	81348	2.66%	0.404%
14	12.540	1740	1743	1748	rBV	105623	100402	3.29%	0.498%
15	12.716	1771	1773	1776	rVB2	62431	52152	1.71%	0.259%
16	12.769	1779	1782	1785	rBV	112042	108890	3.56%	0.541%
17	12.910	1802	1806	1809	rBV	2378833	2004926	65.60%	9.953%
18	13.122	1840	1842	1845	rVB	60754	45497	1.49%	0.226%
19	13.463	1898	1900	1903	rBV2	77569	75456	2.47%	0.375%
20	13.798	1954	1957	1960	rBV4	106724	131860	4.31%	0.655%
21	13.975	1983	1987	1990	rBV	768574	726423	23.77%	3.606%
22	14.063	1999	2002	2005	rVB	191123	173748	5.69%	0.863%
23	14.110	2008	2010	2013	rVB	102189	90609	2.96%	0.450%
24	14.416	2060	2062	2065	rBV	125009	111578	3.65%	0.554%
25	14.716	2111	2113	2116	rVB	96101	84360	2.76%	0.419%
26	15.439	2233	2236	2241	rVB	390444	505430	16.54%	2.509%

Sum of corrected areas: 20143385

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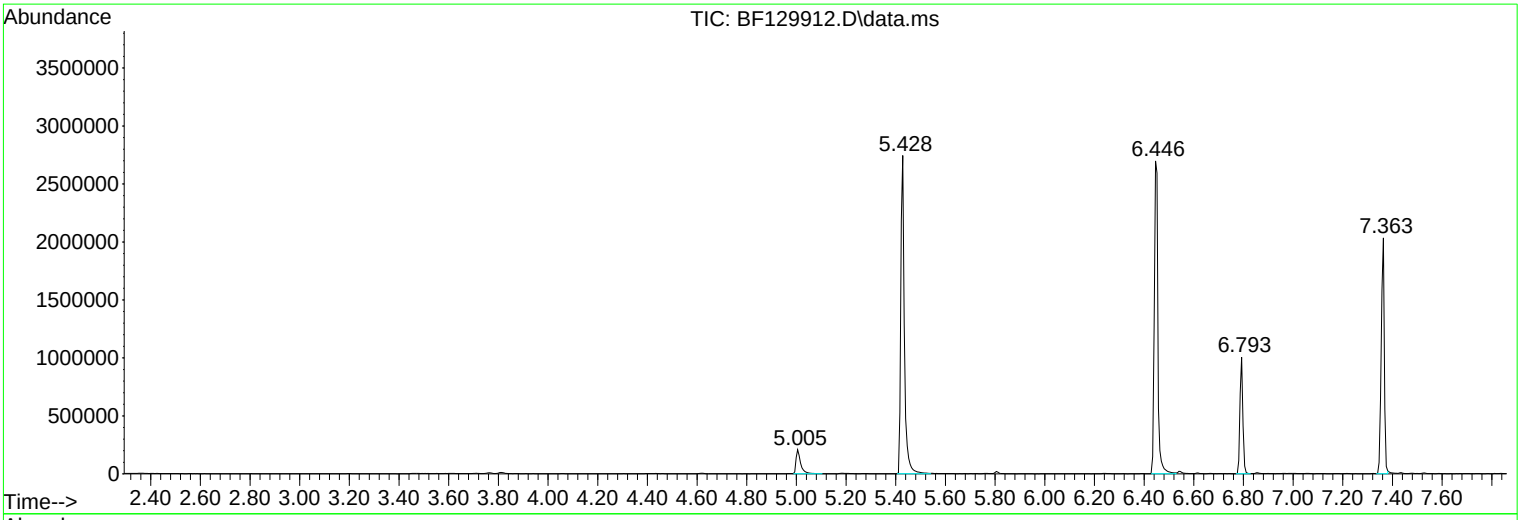
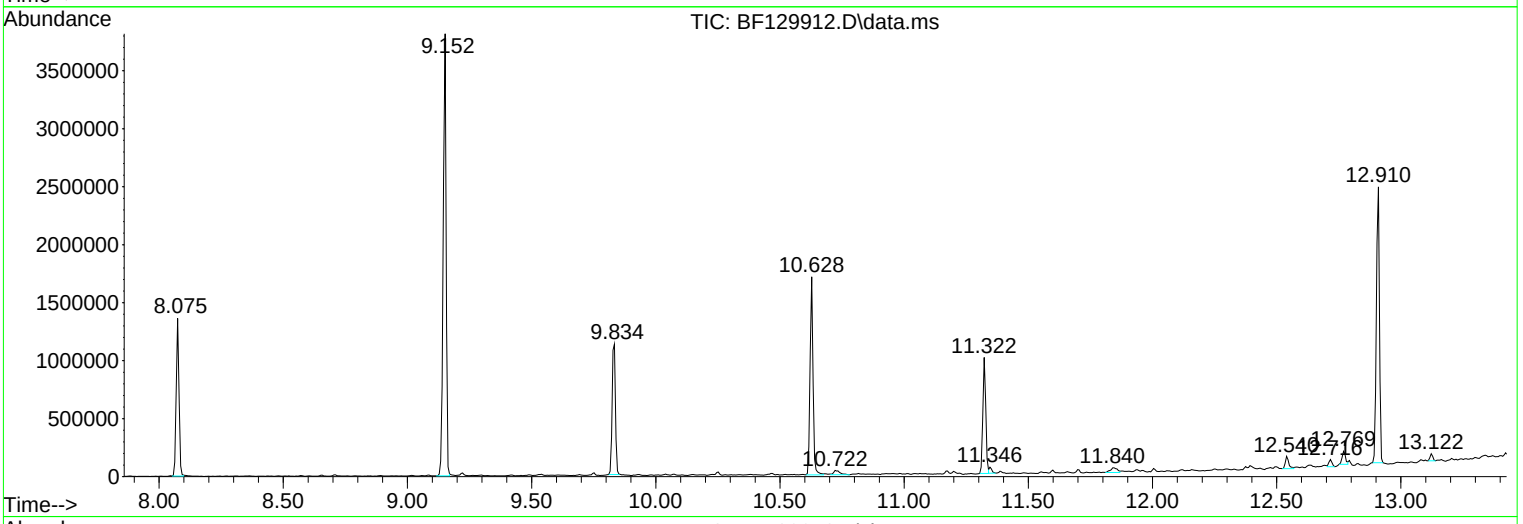
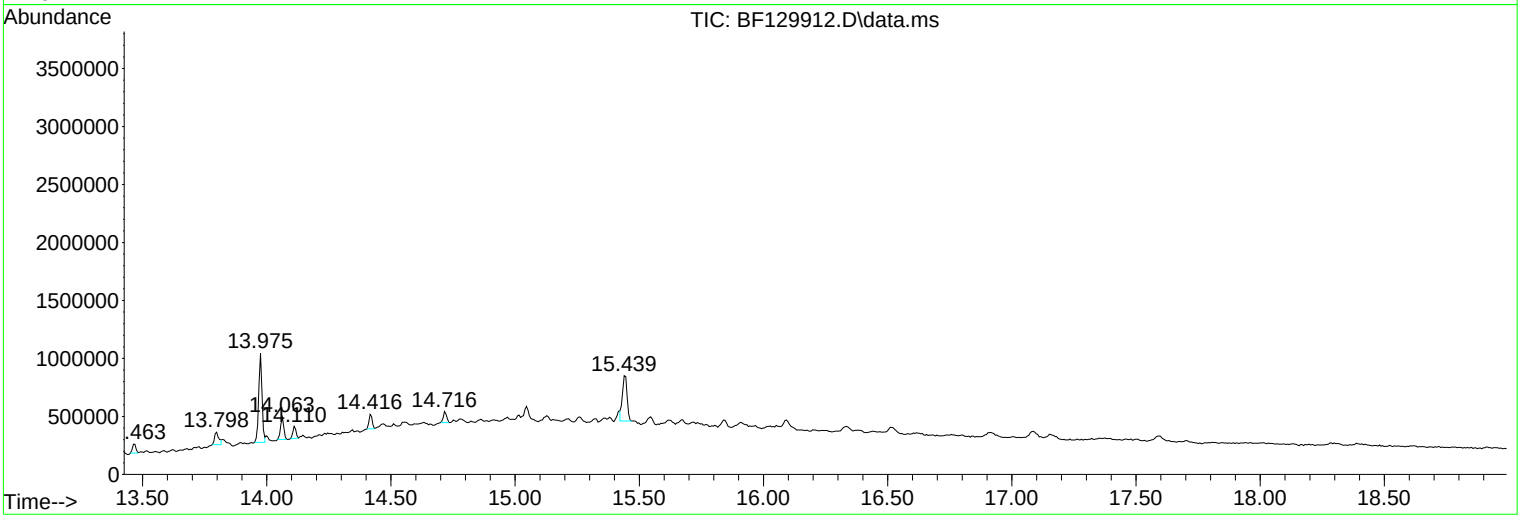
BNA_F
ClientSampleId :
R-70-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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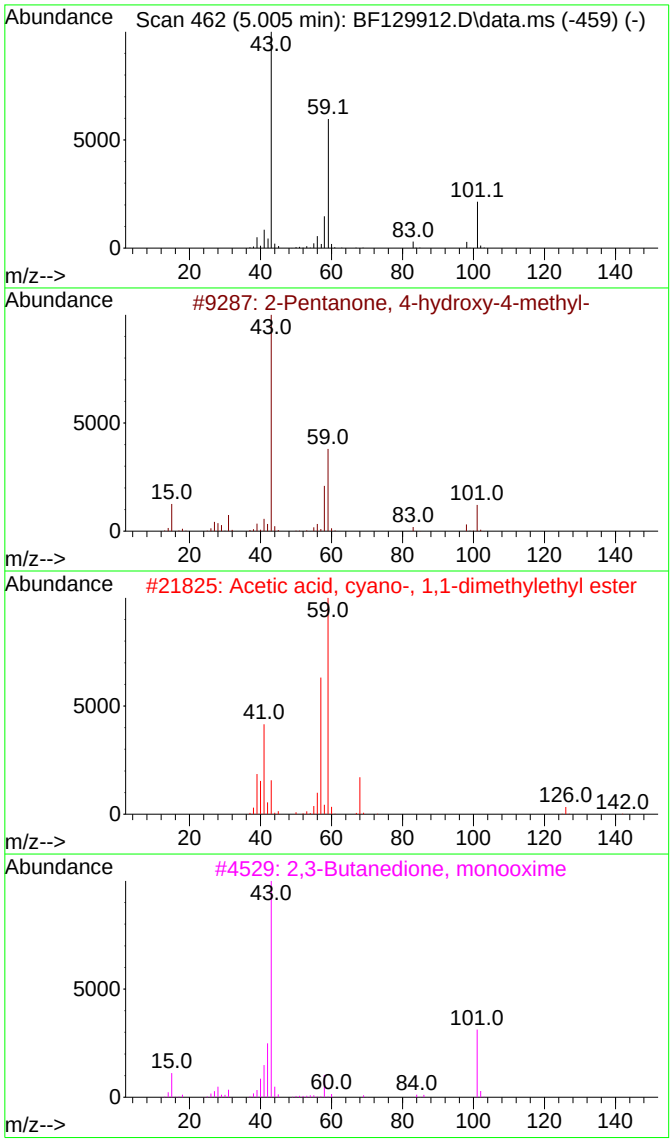
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

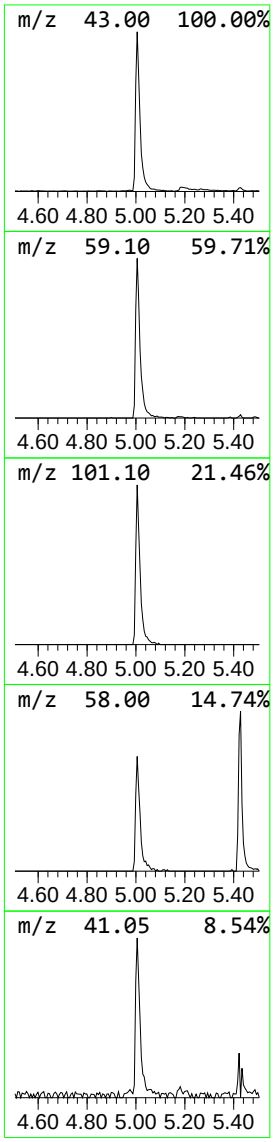
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.005	6.58 ng	268519	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF129912.D
Acq On : 19 Aug 2022 15:12
Operator : CG\JU
Sample : N4225-01
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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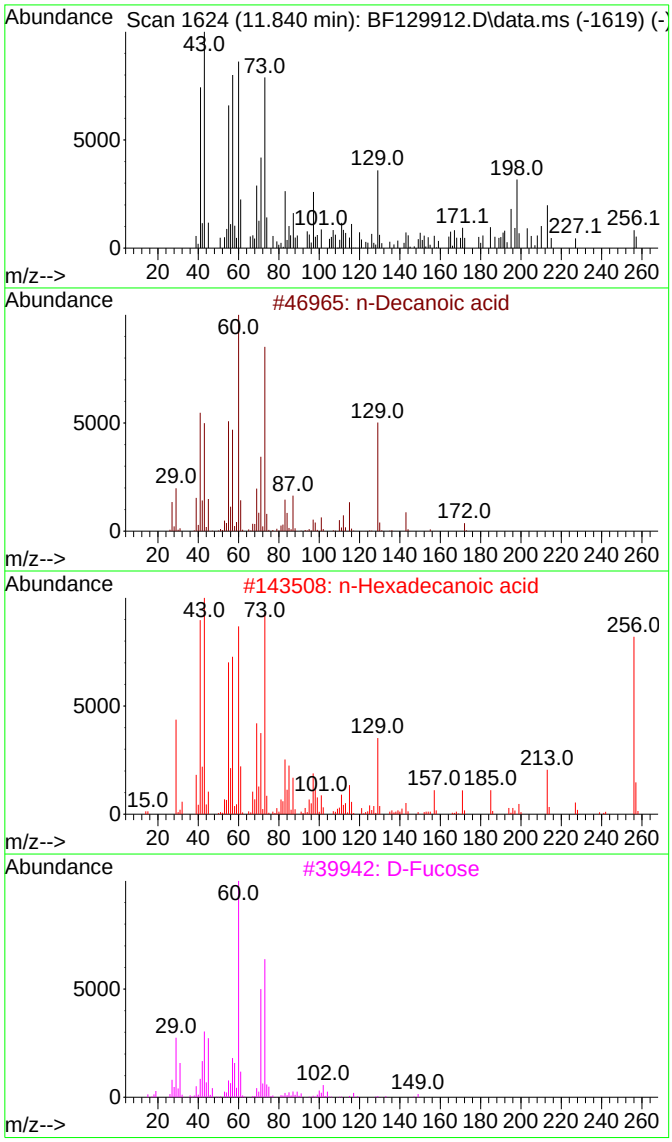
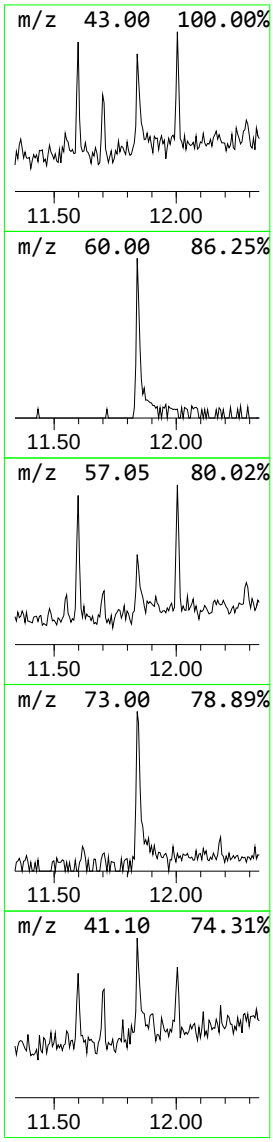
Peak Number 2 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.840	2.02 ng	81348	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	78
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3	D-Fucose	164	C6H12O5	003615-37-0	43
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38





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Misc :
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Instrument :
BNA_F
ClientSampleId :
R-70-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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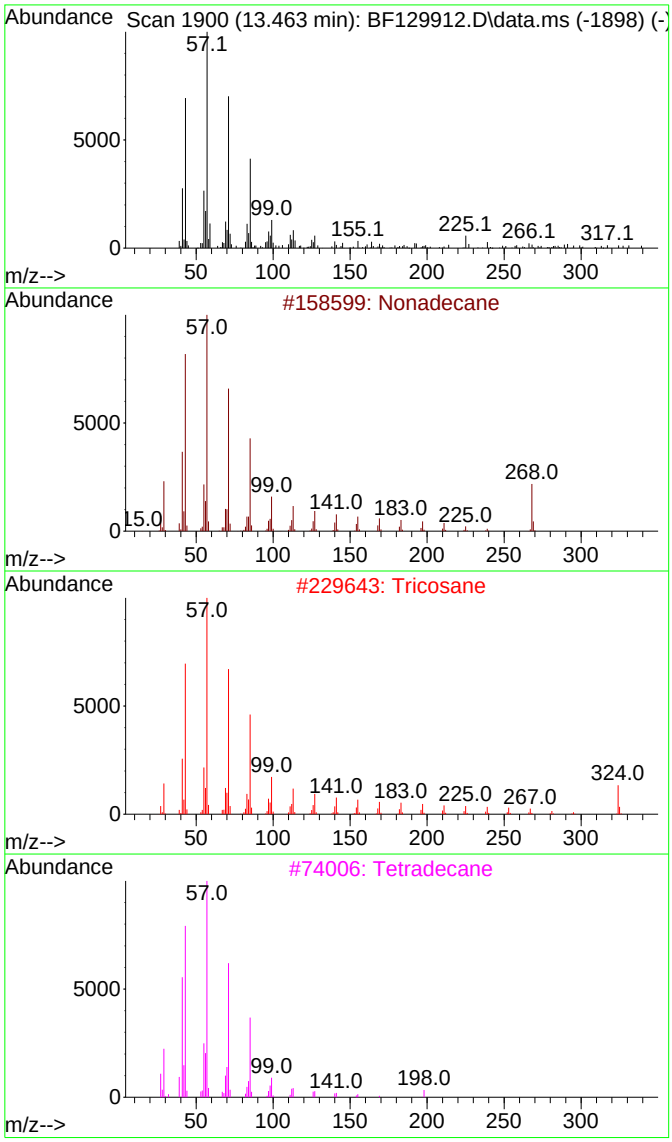
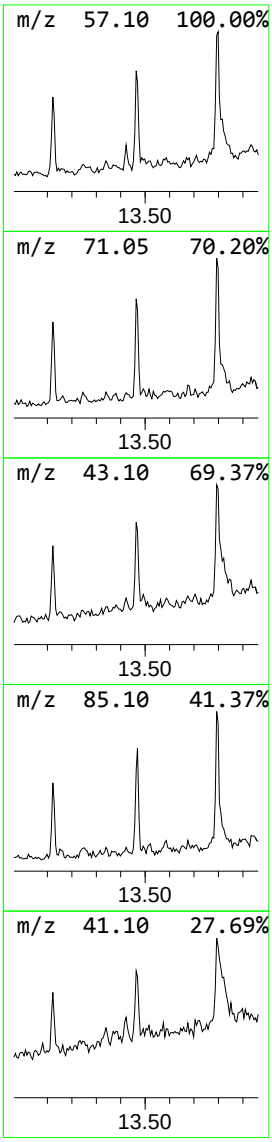
Peak Number 5 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	2.08 ng	75456	Chrysene-d12	13.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Tricosane	324	C23H48	000638-67-5	81
3	Tetradecane	198	C14H30	000629-59-4	81
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	81
5	Pentacosane	352	C25H52	000629-99-2	81





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Data File : BF129912.D
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Misc :
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Instrument :
BNA_F
ClientSampleId :
R-70-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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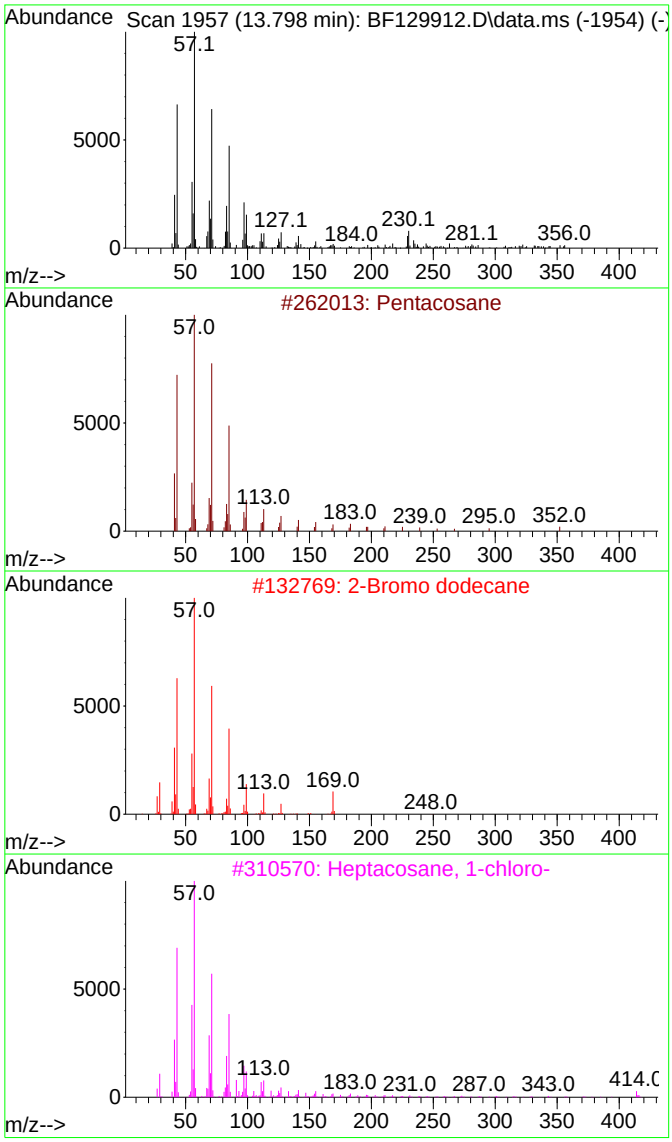
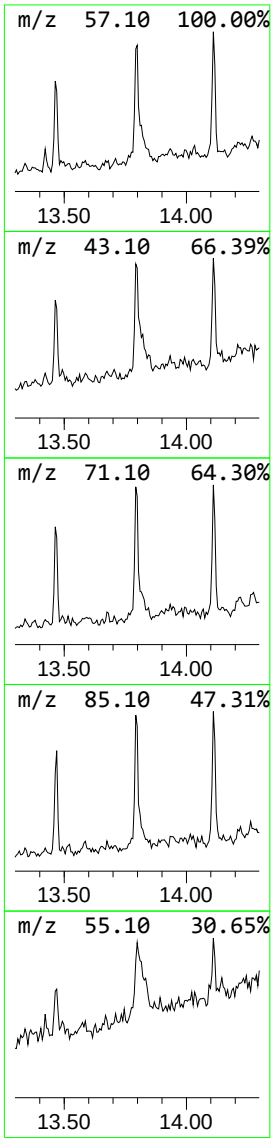
Peak Number 6 Pentacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	3.63 ng	131860	Chrysene-d12	13.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	89
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
4	Tritetracontane	605	C43H88	007098-21-7	83
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081922\
Data File : BF129912.D
Acq On : 19 Aug 2022 15:12
Operator : CG\JU
Sample : N4225-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-70-1

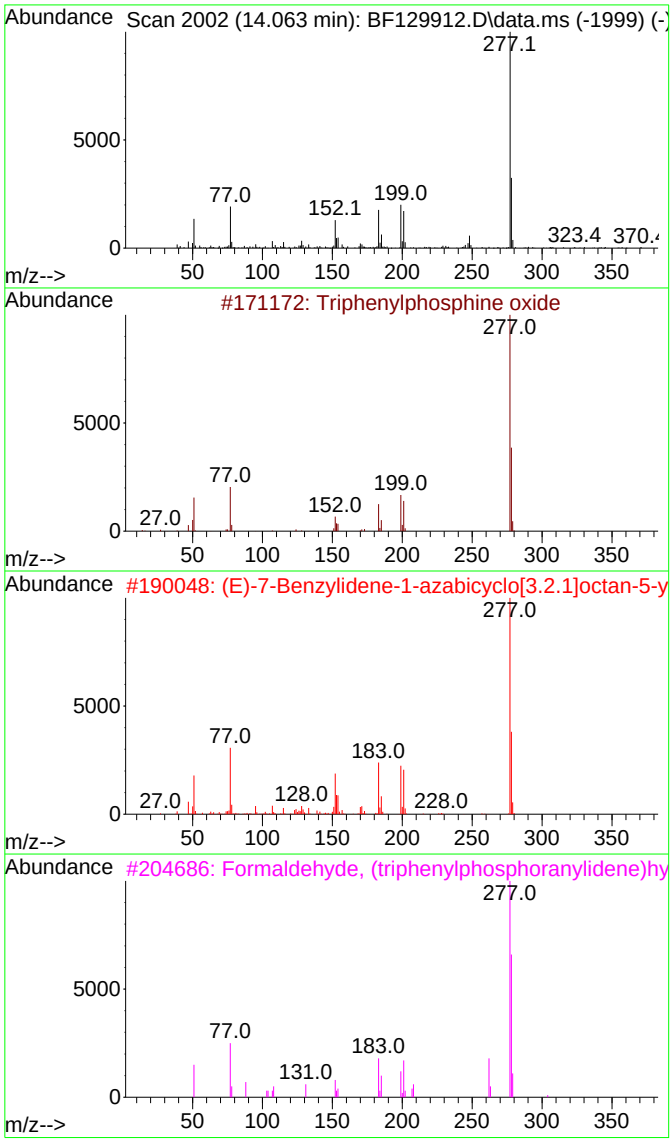
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

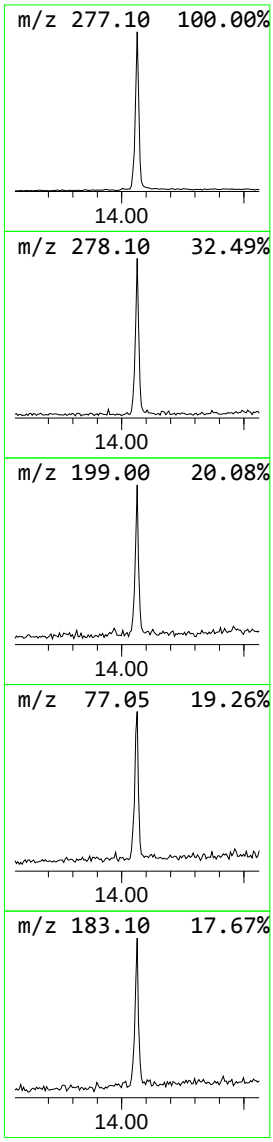
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	4.78 ng	173748	Chrysene-d12	13.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	47
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	1-Methyl-8-piperidinophenazine	277	C18H19N3	021942-85-8	38
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	36





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Instrument :
BNA_F
ClientSampleId :
R-70-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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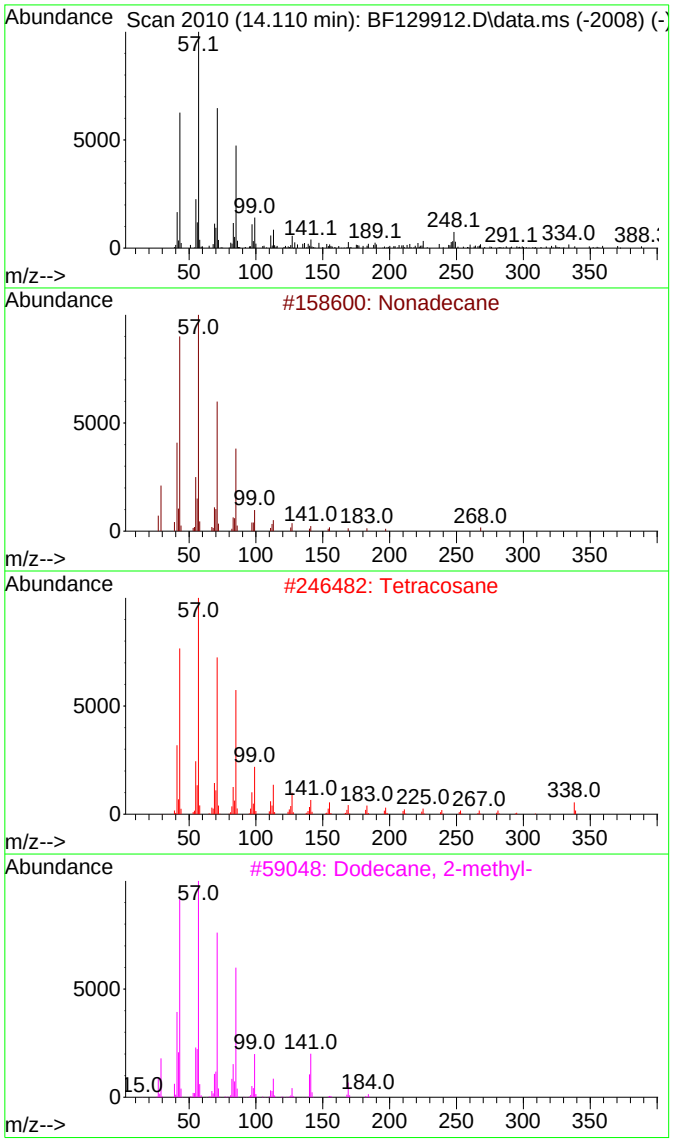
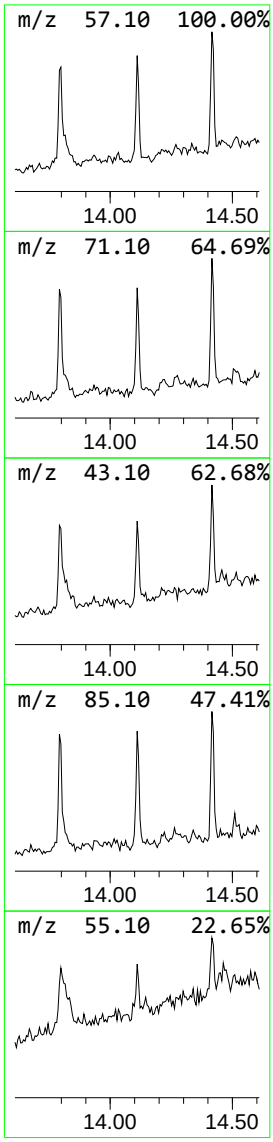
Peak Number 8 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	2.49 ng	90609	Chrysene-d12	13.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	83
5	Hexacosane	366	C26H54	000630-01-3	83





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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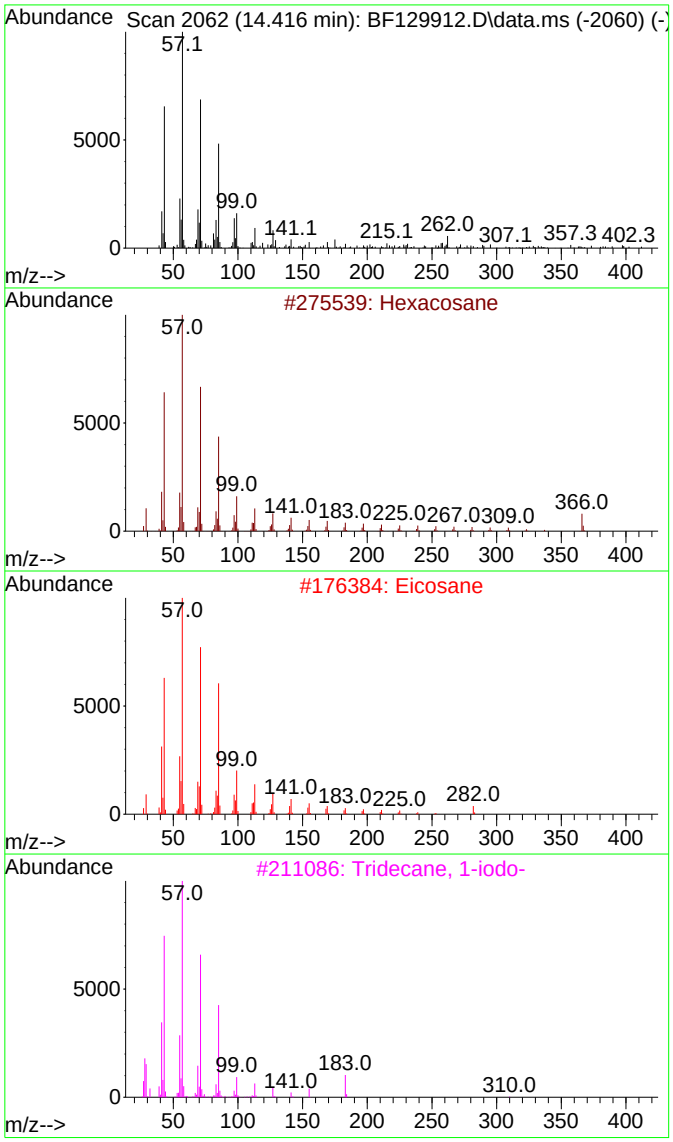
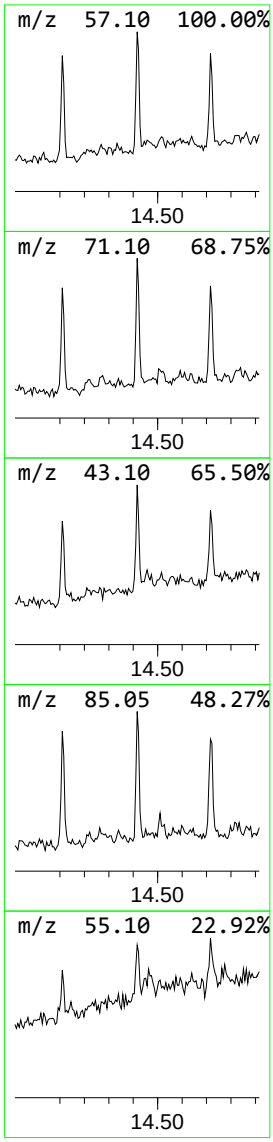
Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.416	3.07 ng	111578	Chrysene-d12	13.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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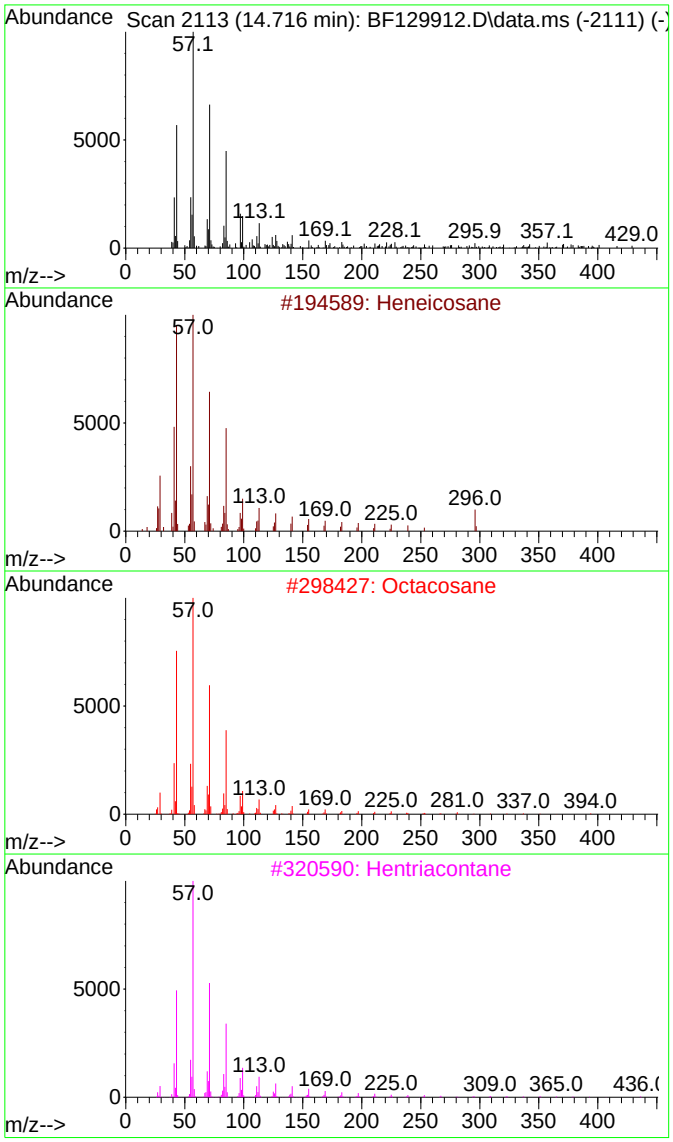
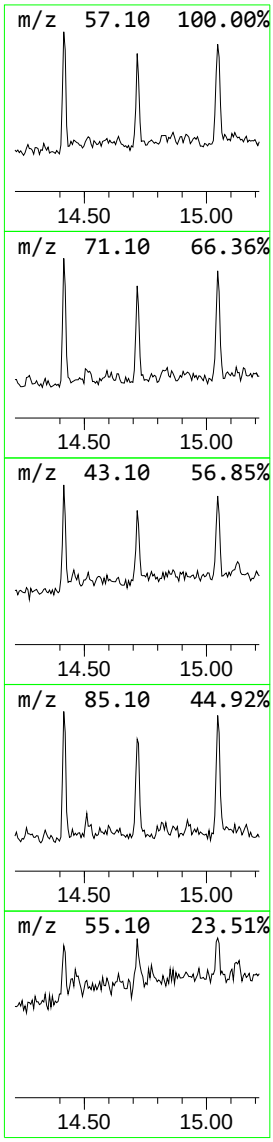
Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.716	3.34 ng	84360	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	3-Methylheptacosane	394	C28H58	014167-66-9	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	89





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.005	6.6	ng	268519	1	6.793	816202	20.0
n-Decanoic acid	11.840	2.0	ng	81348	4	11.322	805328	20.0
Nonadecane	13.463	2.1	ng	75456	5	13.975	726423	20.0
Pentacosane	13.798	3.6	ng	131860	5	13.975	726423	20.0
Triphenylphosph...	14.063	4.8	ng	173748	5	13.975	726423	20.0
Tetracosane	14.110	2.5	ng	90609	5	13.975	726423	20.0
Hexacosane	14.416	3.1	ng	111578	5	13.975	726423	20.0
Heneicosane	14.716	3.3	ng	84360	6	15.445	505430	20.0