LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SP-303-20220428

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_G\Methods\8270-BG040822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053429.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.668	382	388	399	rVB	194868	323697	14.02%	3.599%
2	7.260	652	659	670	rBV	107279	203225	8.80%	2.259%
3	8.100	796	802	809	rVB	83109	142075	6.15%	1.579%
4	9.263	992	1000	1010	rBV	306658	558831	24.20%	6.213%
5	10.913	1273	1281	1290	rVB	98376	183224	7.93%	2.037%
6	13.345	1688	1695	1704	rBV	805519	1253853	54.30%	13.940%
7	14.726	1924	1930	1936	rVB	162392	266392	11.54%	2.962%
8	16.212	2175	2183	2194	rBV	689463	1110405	48.08%	12.345%
9	17.469	2390	2397	2406	rBV	245253	376541	16.31%	4.186%
10	18.650	2589	2598	2608	rBV3	47401	120750	5.23%	1.342%
11	19.719	2773	2780	2789	rVB2	74417	161583	7.00%	1.796%
12	20.072	2834	2840	2849	rBV	1710751	2309330	100.00%	25.674%
13	20.577	2919	2926	2934	rVB2	96063	192234	8.32%	2.137%
14	21.364	3049	3060	3069	rBV2	78447	185955	8.05%	2.067%
15	21.552	3085	3092	3101	rVB2	55347	117080	5.07%	1.302%
16	21.752	3119	3126	3138	rVB	304933	520160	22.52%	5.783%
17	22.251	3201	3211	3219	rBV3	53000	137458	5.95%	1.528%
18	23.285	3378	3387	3396	rBV2	40565	106058	4.59%	1.179%
19	24.489	3586	3592	3602	rVB3	32302	86748	3.76%	0.964%
20	25.047	3677	3687	3700	rVB3	170442	513252	22.23%	5.706%
21	25.928	3829	3837	3845	rVB7	16047	50633	2.19%	0.563%
22	27.620	4120	4125	4134	rVB10	10297	31138	1.35%	0.346%
23	28.777	4314	4322	4324	rBV8	21751	44318	1.92%	0.493%

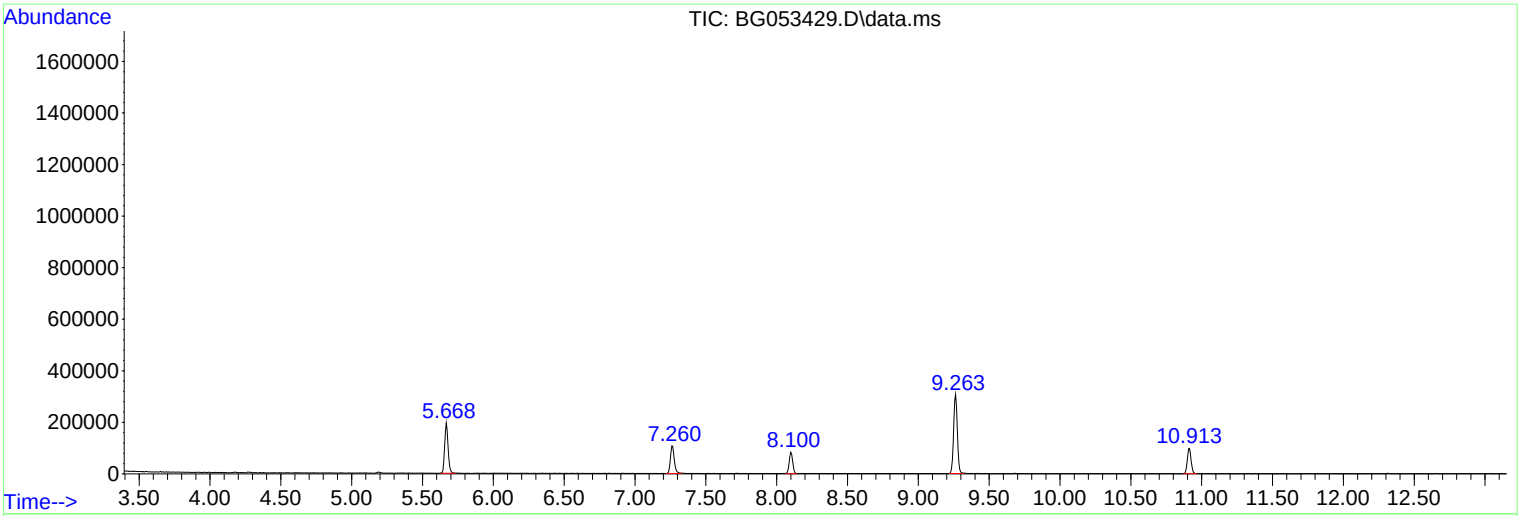
Sum of corrected areas: 8994940

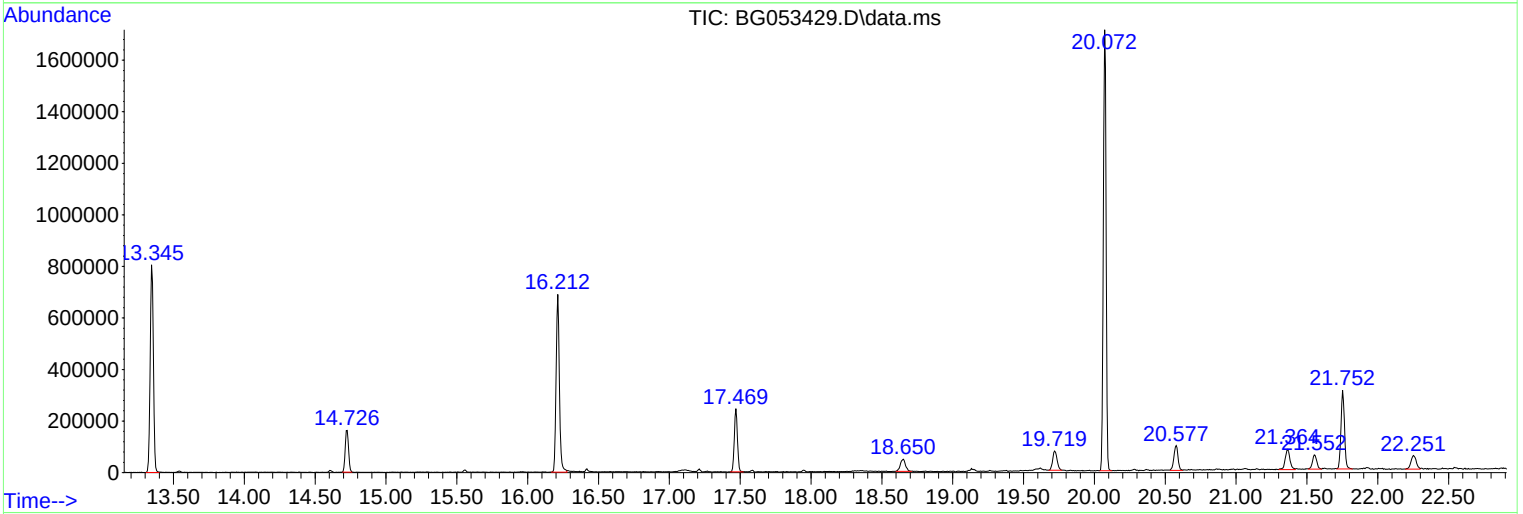
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

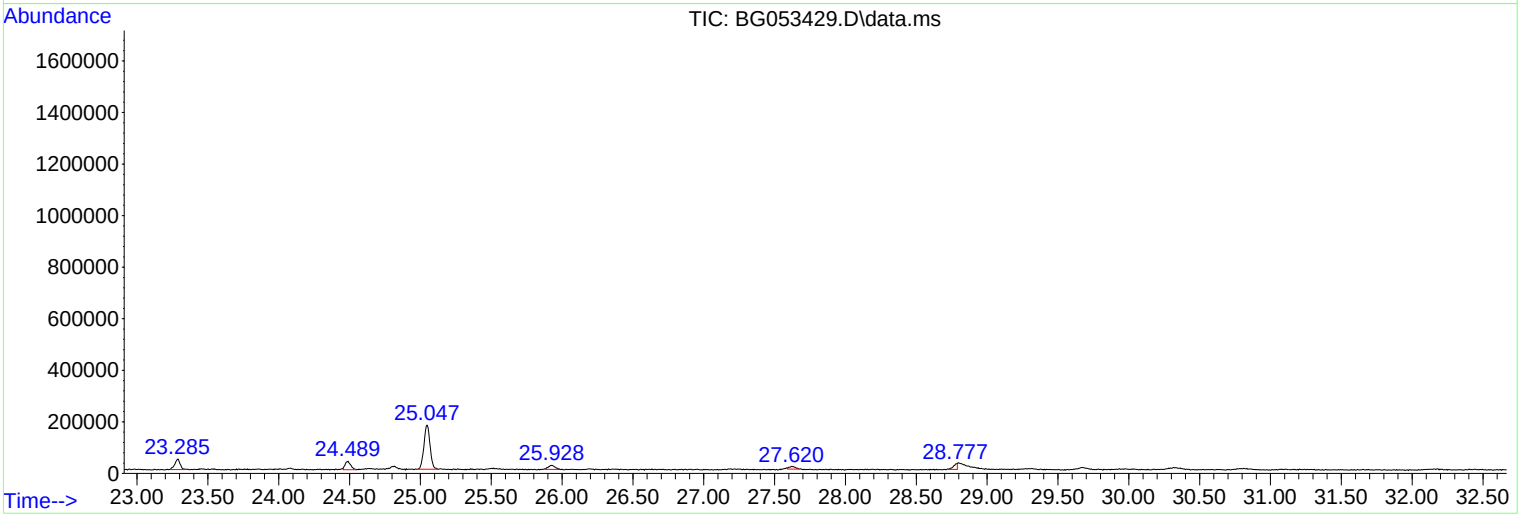
Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

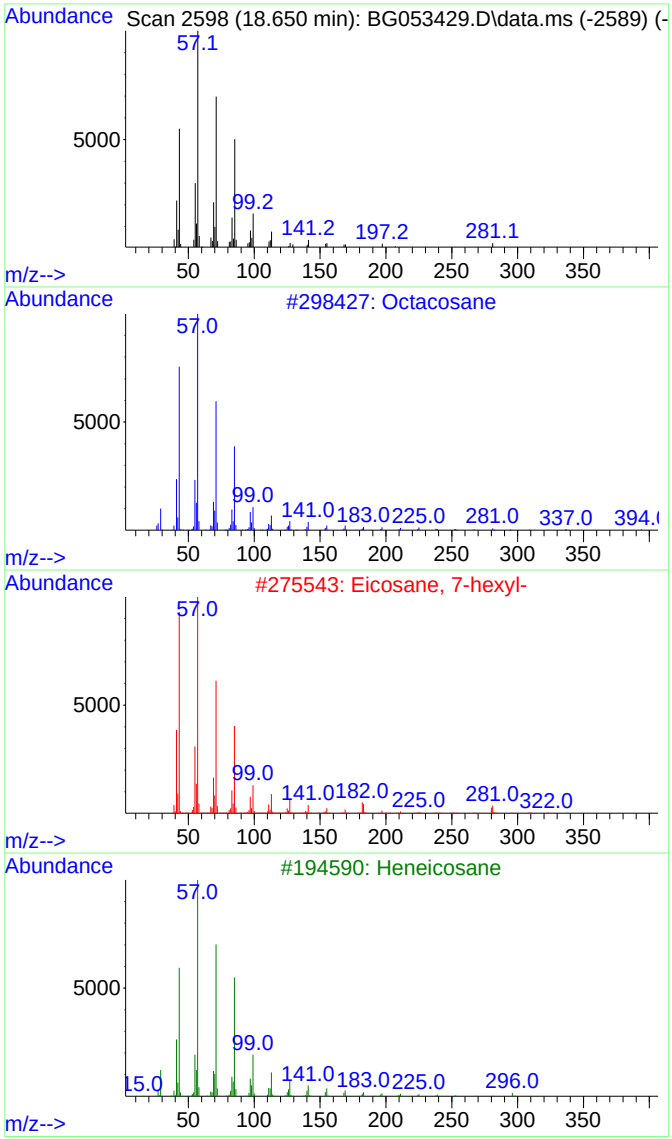
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

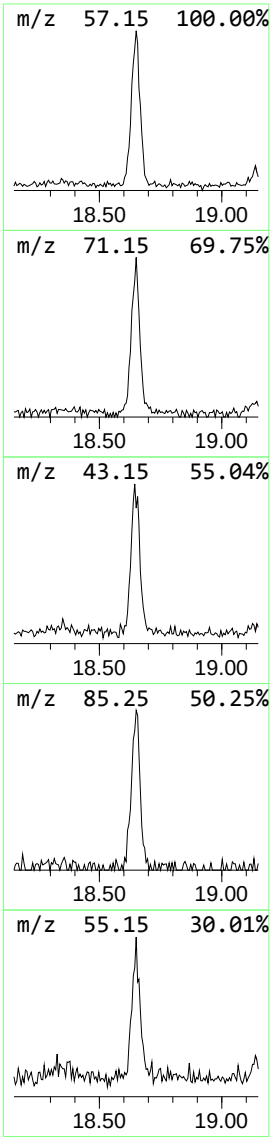
****

Peak Number 1 Eicosane, 7-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.650	6.41 ng	120750	Phenanthrene-d10	17.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Octadecane	254	C18H38	000593-45-3	86
5	Nonadecane	268	C19H40	000629-92-5	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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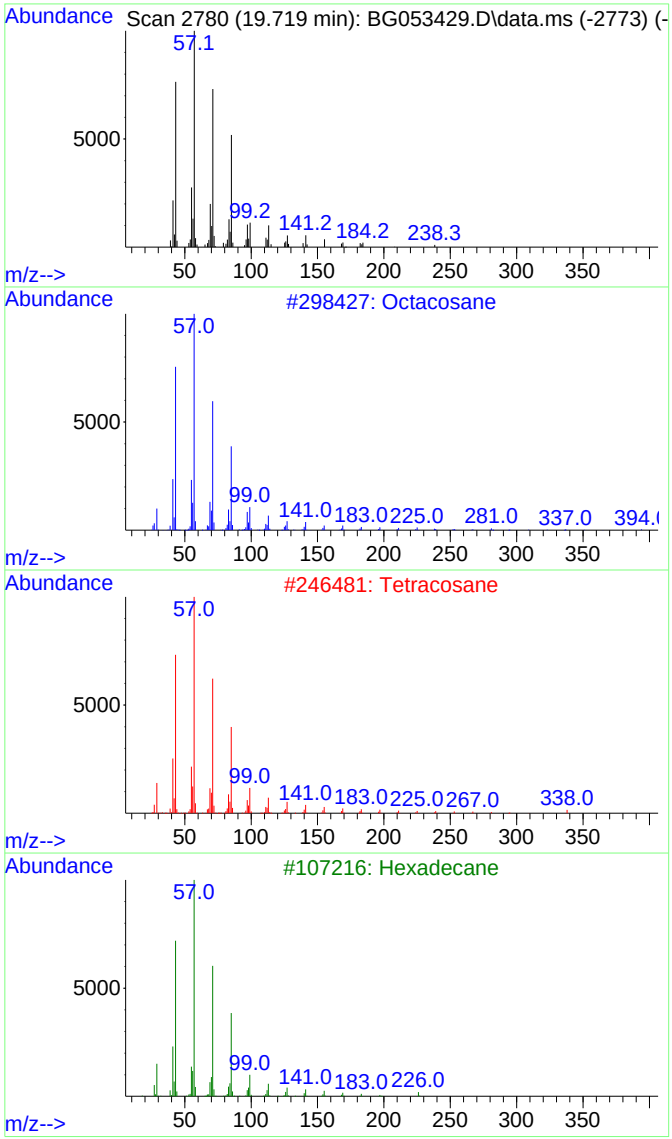
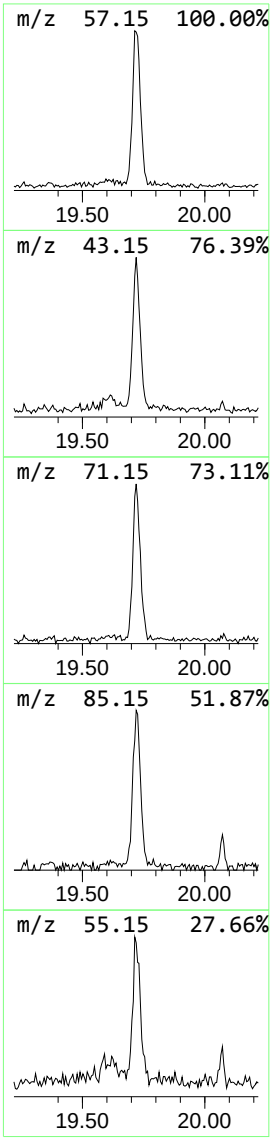
Peak Number 2 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.719	6.21 ng	161583	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hexadecane	226	C16H34	000544-76-3	87
4	Pentadecane	212	C15H32	000629-62-9	87
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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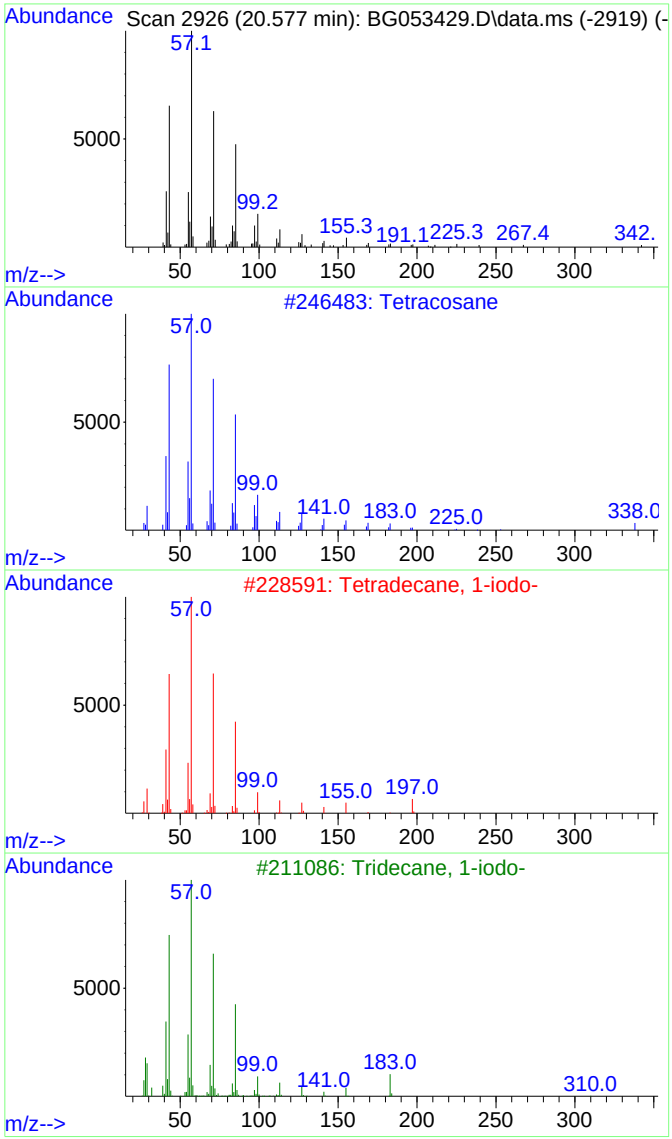
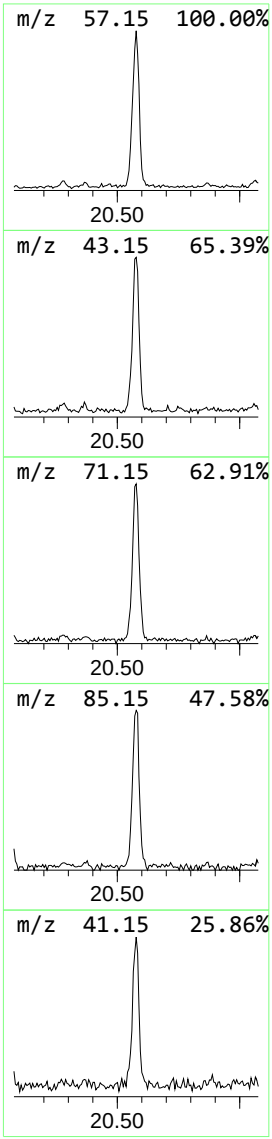
Peak Number 3 Tetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.577	7.39 ng	192234	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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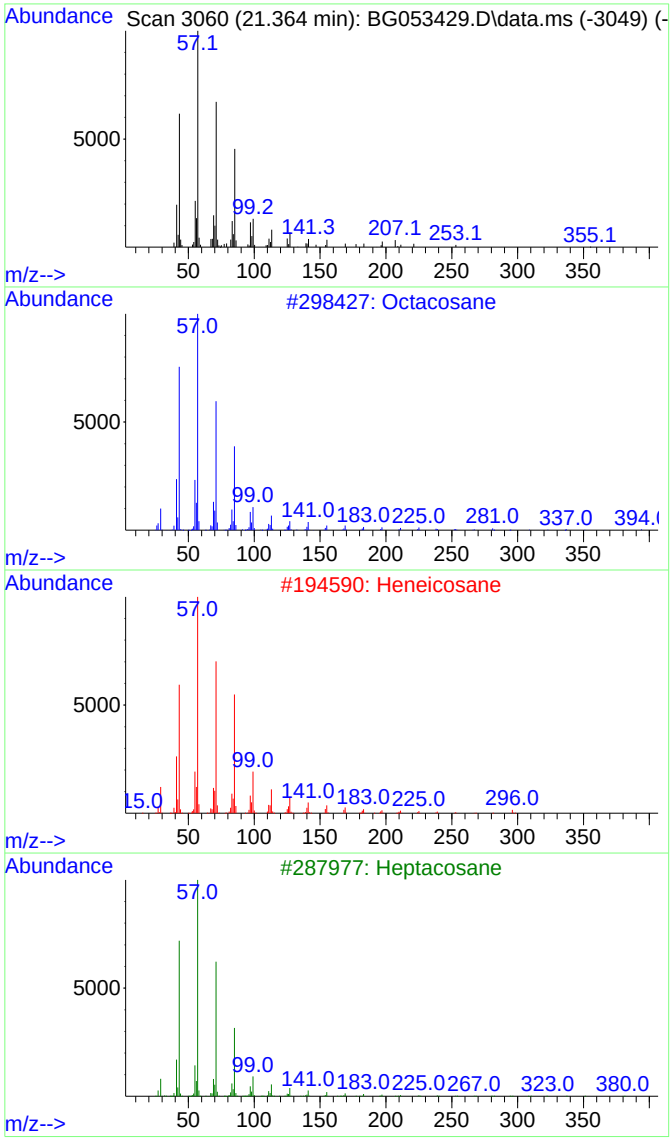
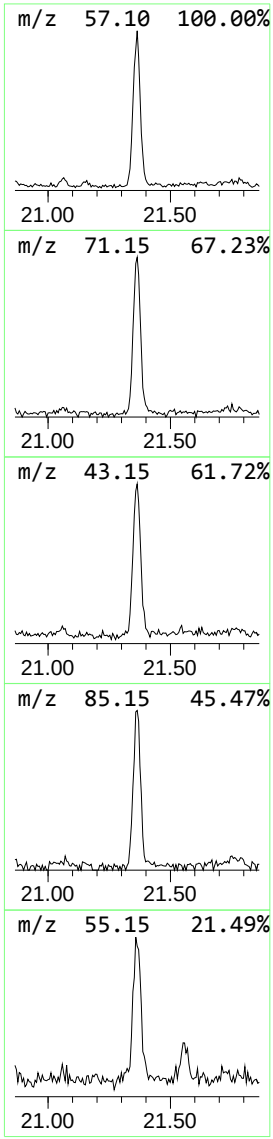
Peak Number 4 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.364	7.15 ng	185955	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

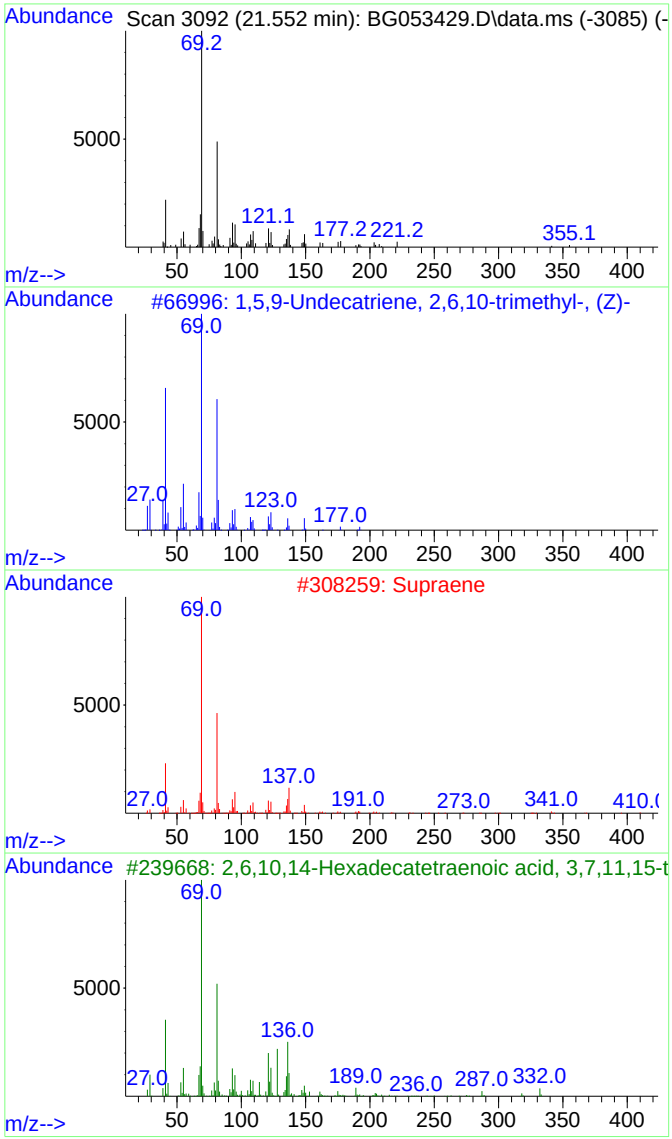
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

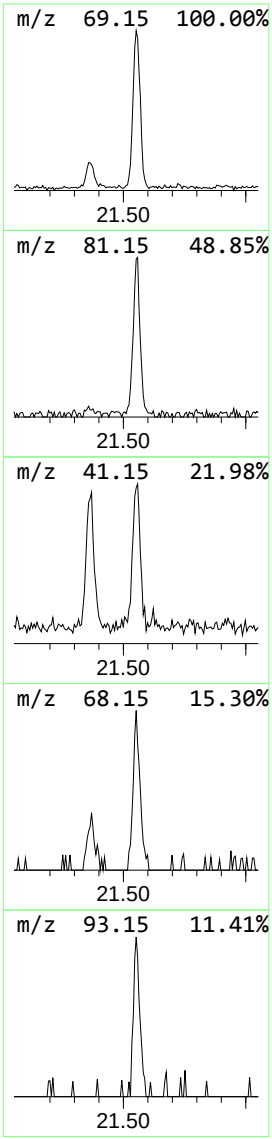
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.552	4.50 ng	117080	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	93
2	Supraene	410	C30H50	007683-64-9	86
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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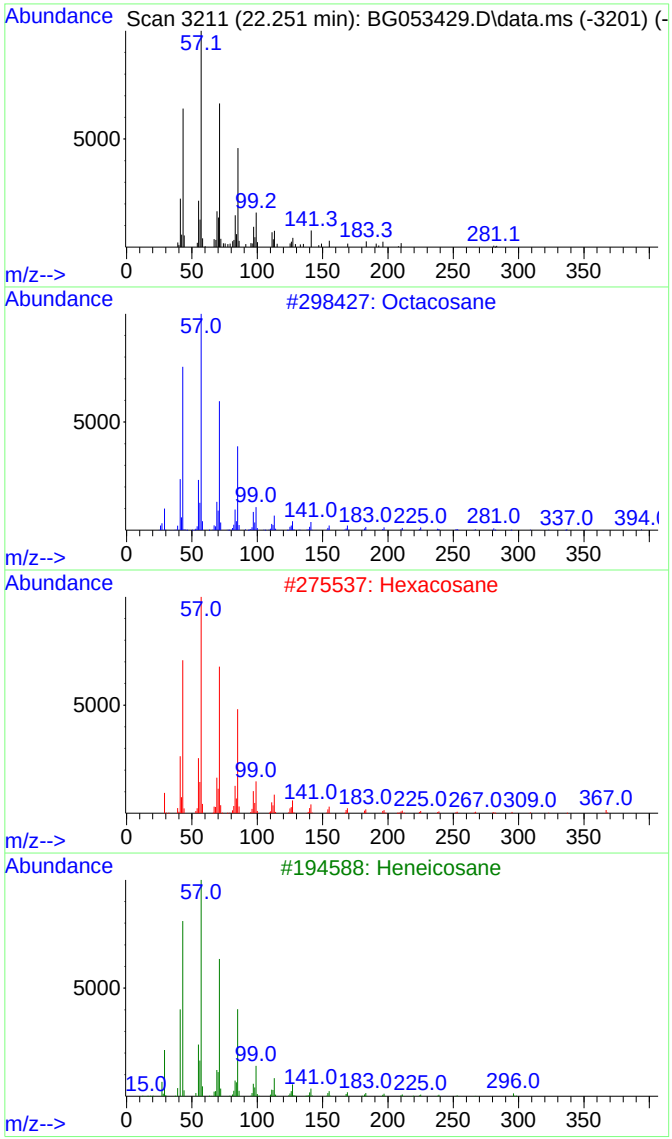
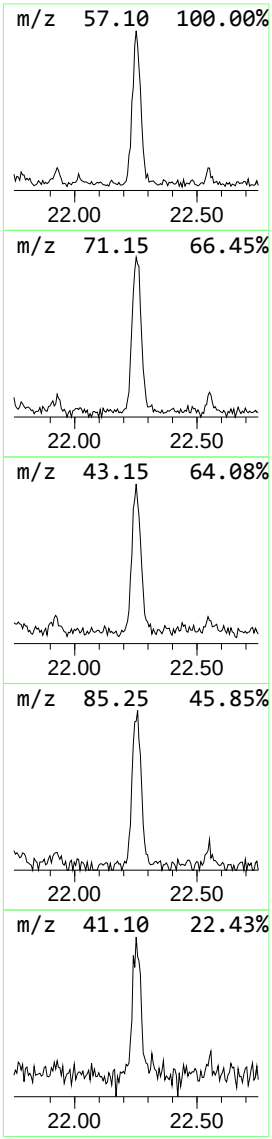
Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.251	5.29 ng	137458	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Tetratetracontane	619	C44H90	007098-22-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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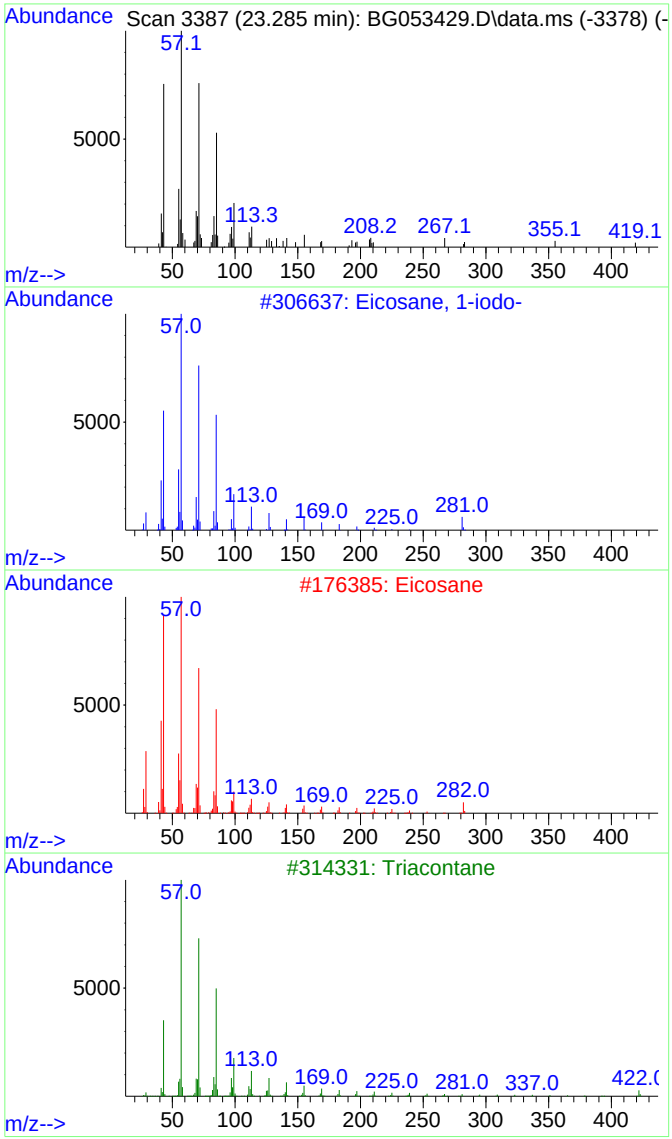
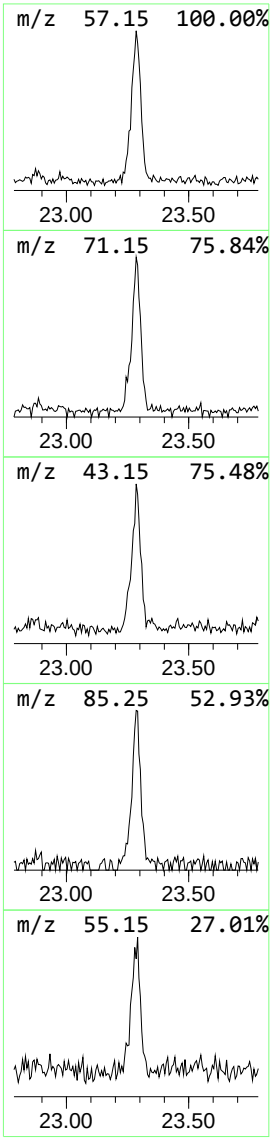
Peak Number 7 Eicosane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.285	4.08 ng	106058	Chrysene-d12	21.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Triacontane	422	C30H62	000638-68-6	86
4	Hexacosane	366	C26H54	000630-01-3	83
5	Octacosane	394	C28H58	000630-02-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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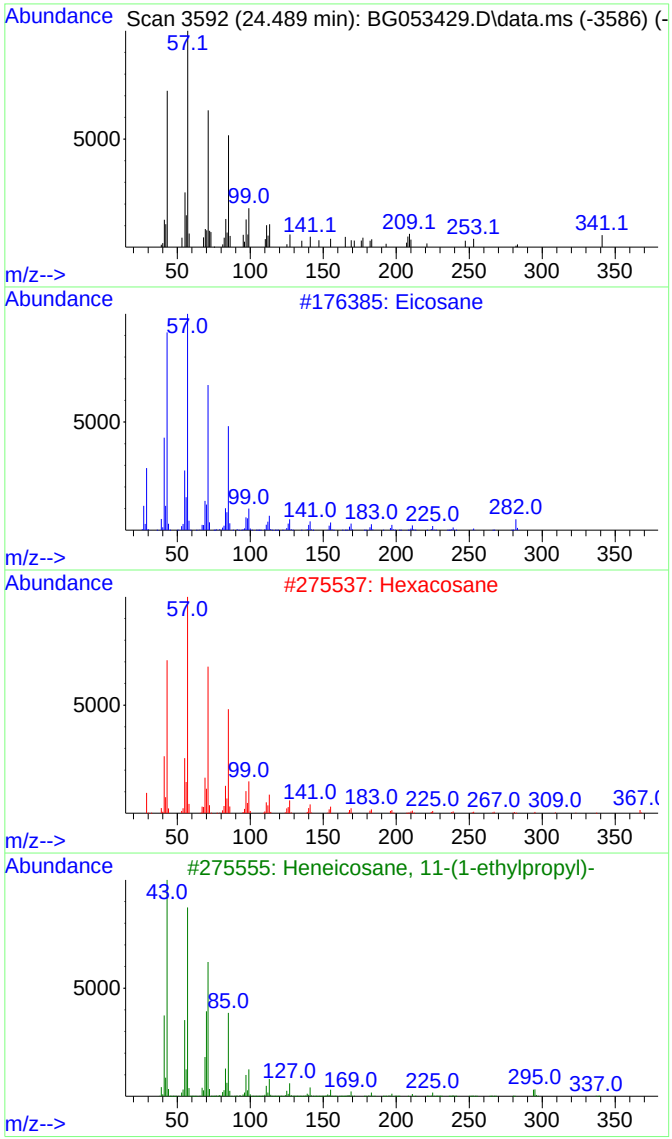
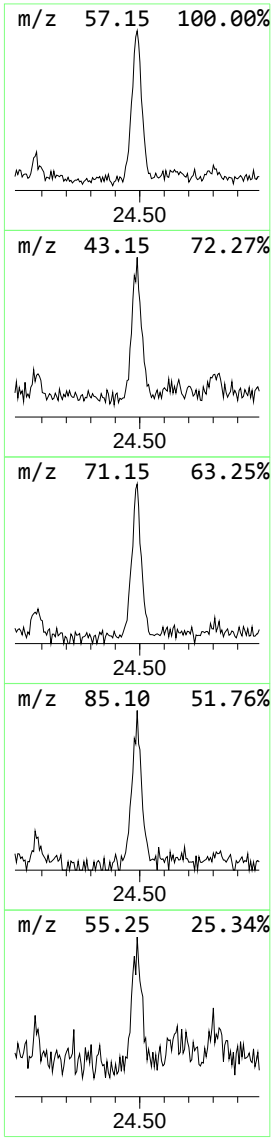
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.489	3.38 ng	86748	Perylene-d12	25.047

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4	Tetracosane	338	C24H50	000646-31-1	80
5	Heptacosane	380	C27H56	000593-49-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050422\
Data File : BG053429.D
Acq On : 4 May 2022 13:50
Operator : CG/JU
Sample : N2622-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20220428

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
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
Eicosane, 7-hexyl-	18.650	6.4	ng	120750	4	17.469	376541	20.0
Octacosane	19.719	6.2	ng	161583	5	21.752	520160	20.0
Tetracosane	20.577	7.4	ng	192234	5	21.752	520160	20.0
Heneicosane	21.364	7.2	ng	185955	5	21.752	520160	20.0
1,5,9-Undecatri...	21.552	4.5	ng	117080	5	21.752	520160	20.0
Hexacosane	22.251	5.3	ng	137458	5	21.752	520160	20.0
Eicosane, 1-iodo-	23.285	4.1	ng	106058	5	21.752	520160	20.0
Eicosane	24.489	3.4	ng	86748	6	25.047	513252	20.0